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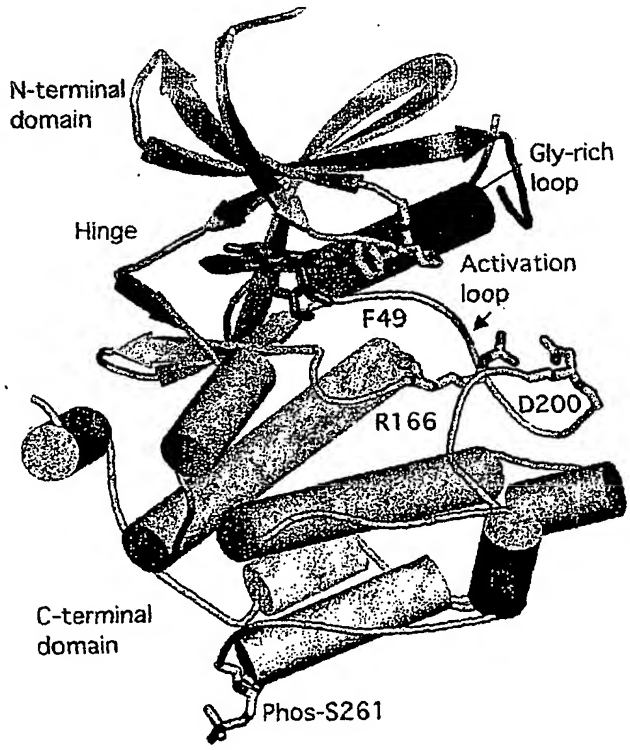

(57) Abstract: The present invention relates to the X-ray analysis of crystalline molecules or molecular complexes of human Pim-1. The present invention also relates to Pim-1-like binding pockets. The present invention provides a computer comprising a data storage medium encoded with the structure coordinates of such binding pockets. This invention also relates to methods of using the structure coordinates to solve the structure of homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen for and design compounds, including inhibitory compounds, that bind to Pim-1 protein, Pim-1 protein complexes, or homologues thereof. The invention also relates to crystallizable compositions and crystals comprising Pim-1 protein, Pim-1 protein complexes with adenosine, staurosporine or 2-(4-morpholinyl)-8-phenyl-4H-1-benzopyran-4-one and methods to produce these crystals.

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CRYSTAL STRUCTURES OF HUMAN PIM-1 KINASE PROTEIN COMPLEXES AND BINDING POCKETS THEREOF, AND USES THEREOF IN DRUG DESIGN

[0001] This application claims benefit of United States Provisional Application No. 60/460,843, titled CRYSTAL STRUCTURE OF HUMAN PIM-1 KINASE PROTEIN AND BINDING POCKETS THEREOF, filed April 4, 2003, and United States Provisional Application No: 60/552,526 titled CRYSTAL STRUCTURE OF HUMAN PIM-1 KINASE PROTEIN COMPLEXES AND BINDING POCKETS THEREOF, AND USES THEREOF IN DRUG DESIGN, filed March 12, 2004, the disclosures of which are incorporated herein by reference.

TECHNICAL FIELD OF INVENTION

[0002] The present invention relates to the X-ray analysis of crystalline molecules or molecular complexes of human Pim-1. The present invention also relates to Pim-1-like binding pockets. The present invention provides a computer comprising a data storage medium encoded with the structure coordinates of such binding pockets. This invention also relates to methods of using the structure coordinates to solve the structure of homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen for and design

compounds, including inhibitory compounds, that bind to Pim-1 protein, Pim-1 protein complexes, or homologues thereof. The invention also relates to crystallizable compositions and crystals comprising Pim-1 protein, Pim-1 protein complexes with adenosine, staurosporine or 2-(4-morpholinyl)-8-phenyl-4H-1-benzopyran-4-one and methods to produce these crystals.

BACKGROUND OF THE INVENTION

[0003] Pim-1 is an oncogene-encoded serine/threonine kinase primarily expressed in hematopoietic and germ cell lines. The *Pim-1* oncogene was originally identified as a preferred site for proviral integration of the slow transforming Maloney murine Leukemia Virus (MuLV)-induced in lymphoblastic T-cells and is associated with multiple cellular functions such as proliferation, survival, differentiation, apoptosis and tumorigenesis (Wang et al., *J. Vet. Sci.* 2: 167-179 (2001)). Direct evidence for the oncogenic potential of the *Pim-1* gene comes from the study of transgenic mice in which overexpression of *Pim-1* produces a low but spontaneous rate of tumor incidence (Domen et al., *Leukemia* 7 (Suppl. 2):S108-112 (1993)). These mice are highly susceptible to chemical carcinogens, X-ray radiation and MuLV-induced lymphomagnesis. In most cases, this correlated with the upregulation of *c-* or *N-myc* genes suggesting synergism between the *Pim-1* and *myc* genes in the development of lymphomas (Breuer et al., *Cancer Res.* 51: 958-963 (1991); van Lohuizen et al., *Cell* 56: 673-682 (1989)). *Pim-1* knockout mice did not show any obvious phenotype suggesting *in vivo* functional redundancy of this highly conserved oncogene (Domen et al., *J. Exp. Med.* 178: 1665-1673 (1993)).

[0004] Since the initial report of the cloning of mouse *Pim-1* gene (Selten et al., *Cell*, 46: 603-611 (1986)), *Pim-1* has been cloned from human, rat, bovine and zebrafish cDNA libraries (Wang et al., *J. Vet. Sci.* 2: 167-179 (2001)). In humans, the *Pim-1* gene is expressed mainly in the developing fetal liver and spleen (Amson et al., *Proc. Natl. Acad. Sci.* U.S.A. 86: 8857-8861 (1989)) and in hematopoietic malignancies (Nagarajan et al., *Proc. Natl. Acad. Sci.* U.S.A. 83: 2556-2560 (1986); Meeker et al., *Oncogene Res.* 1: 87-101 (1987)). Two homologues of the *Pim-1* gene, *pim-2* (Allen et al., *Oncogene 15*: 1133-1141 (1997); van der Lugt et al., *Embo J.* 14:

2536-2544 (1995)) and *pim-3/kid-1* (Feldman et al., *J. Biol. Chem.* 273: 16535-16543 (1998)) have also been identified.

[0005] The expression of Pim-1 is tightly regulated and is induced by cytokines, mitogens and hormones: IL-2, IL-3, IL-5, IL-6, IL-7, IL-9, IL-12 and IL-15, granulocyte-macrophage colony-stimulating factor (GM-CSF), erythropoietin, ConA, PMA, interferon-γ and prolactin (Wang et al., *J. Vet. Sci.* 2: 167-179 (2001)). The JAK/STAT pathway may be one of several signaling pathways that mediate Pim-1 expression (Nagata et al., *Leukemia* 11(Suppl 3): 435-438 (1997); Sakai and Kraft, *J. Biol. Chem.* 272: 12350-12358 (1997); O'Farrell et al., *Blood* 87: 3655-3668 (1996); Kumenacker et al., *J. Neuroimmunol.* 113: 249-259 (2001)). However, results from a study by Krishnan and colleagues (Krishnan et al., *Endocrine 20*: 123-130 (2003)) do not support a role for the JAK/STAT signaling pathway, but, instead, implicate AKT activation as a component of prolactin-induced *Pim-1* transcription. Also, mitogen-activated protein kinase (MAPK) and phosphatidylinositol-3-kinase (PI-3-kinase) pathways may mediate prolactin-induced Pim-1 expression (Kumenacker et al., *supra*).

[0006] The human *Pim-1* gene encodes a 313 amino acid serine-threonine kinase (Padma et al., *Cancer Res.* 51: 2486-2489 (1991); Hoover et al., *J. Biol. Chem.* 266: 14018-14023 (1991)) and is associated with multiple cellular functions such as proliferation, differentiation, apoptosis and tumorigenesis (Wang et al., *J. Vet. Sci.* 2: 167-179 (2001)). Several cellular substrates of Pim-1 have been identified, including the transcription factors cMyb (Winn et al., *Cell Cycle 2*: 258-262 (2003)) and NFATc1 (Rainio et al., *J. Immunol.* 168: 1524-7 (2002)), transcriptional co-activator of cMyb p100 (Leverson et al., *Mol. Cell* 2: 417-425 (1998)), phosphatases Cdc25A (Mochizuki et al., *J. Biol. Chem.* 274: 18659-18666 (1999)), and PTPU2S (Wang et al., *J. Biol. Chem.* 274: 18659-18666 (2001)), Pim-1 associated protein 1 (PAP-1) (Maita et al., *Eur. J. Biochem.* 267: 5168-5178 (2000)), cell-cycle inhibitor p21/WAF1 (Wang et al., *Biochem. Biophys. Acta* 1593: 45-55 (2002)), heterochromatin protein 1 (HP1) (Koike et al., *FEBS Lett.* 467: 17-21 (2000)), TRAF2/SNX6 (Ishibashi et al., *FEBS Lett.* 506: 33-38 (2001)) and nuclear mitotic apparatus (Bhattacharya et al., *Chromosoma* 111: 80-95 (2002)).

[0007] The consensus sequence for Pim-1 substrate recognition is Lys/Arg-Lys/Arg-Arg-Lys/Arg-Leu-Ser/Thr-X (SEQ ID NO:1), where X is an amino acid with a small side chain (Friedmann et al., *Arch. Biochem. Biophys.* 298: 594-601 (1992); Palaty et al., *Biochem. Cell. Biol.* 75: 153-162 (1997)). A detailed analysis of the autophosphorylation sites of Xenopus Pim-3 (previously incorrectly identified as Pim-1) has also been reported (Palaty et al., *J. Biol. Chem.* 272: 10514-10521 (1997)).

[0008] Due to the lack of structural information about Pim-1, the detailed mechanism of the protein is not known. Without such structural information and knowledge of the mechanism, the progress in designing drugs as specific inhibitors is impeded. Structural information on the unique features of the active site of Pim-1 would facilitate drug discovery and the treatment of cancer.

SUMMARY OF THE INVENTION

[0009] The present invention provides for the first time the crystal structures of Pim-1-adenosine, Pim-1 staurosporine and Pim-1-LY294002 (2-(4-morpholinyl)-8-phenyl-4H-1-benzopyran-4-one) complexes. These structures present a rationale for the structure-based design of small molecule Pim-1 inhibitors as therapeutic agents, thus addressing the need for novel drugs for the treatment of cancer.

[0010] The present invention also provides molecules comprising Pim-1 binding pockets, or Pim-1-like binding pockets that have similar three-dimensional shapes. In one embodiment, the molecules are Pim-1 protein complexes or homologues thereof. In another embodiment, the molecules are in crystalline form.

[0011] The invention also provides crystallizable compositions and crystal compositions comprising phosphorylated Pim-1 kinase, complexes thereof, or homologues thereof.

[0012] The invention provides a computer comprising a machine-readable storage medium, comprising a data storage material encoded with machine-readable data, wherein the data defines the Pim-1 or Pim-1-like binding pocket or protein according to the structure coordinates of Figure 1A, 2A, or 3A. Such storage medium when read and utilized by a computer programmed with appropriate software can display, on a computer screen or similar viewing device, a three-dimensional graphical

representation of such binding pockets. In one embodiment, the structure coordinates of said binding pocket or protein are produced by homology modeling of at least a portion of the coordinates of Figures 1A, 2A or 3A.

[0013] The invention also provides methods for designing, selecting, evaluating and identifying and/or optimizing compounds which bind to the molecules or molecular complexes or their binding pockets. Such compounds are potential inhibitors of Pim-1 or its homologues.

[0014] The invention also provides a method for determining at least a portion of the three-dimensional structure of molecules or molecular complexes which contain at least some structurally similar features to Pim-1, particularly Pim-1 homologues. This is achieved by using at least some of the structure coordinates obtained from the Pim-1 protein.

BRIEF DESCRIPTION OF THE FIGURES

[0015] The following abbreviations are used in Figures 1A, 2A and 3A:

[0016] "Atom type" refers to the element whose coordinates are measured. The first letter in the column defines the element.

[0017] "Resid" refers to the amino acid residue in the molecular model.

[0018] "X, Y, Z" define the atomic position of the element measured.

[0019] "B" is a thermal factor that measures movement of the atom around its atomic center.

[0020] "Occ" is an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i.e., the same position, in the molecules.

[0021] "Mol" refers to a molecule in the asymmetric unit. Mol A, W and Z are Pim-1 protein, water and adenosine, respectively.

[0022] Residue "PSR", "ADE", STO" and "LY2" represent phosphorylated serine, adenosine, staurosporine and LY294002, respectively.

[0023] Figure 1 (1A-1 to 1A-42) lists the atomic structure coordinates in Protein Data Bank (PDB)-like form for phosphorylated human Pim-1 in complex with adenosine (Pim-1-adenosine complex), as derived by X-ray diffraction from a crystal of the complex. The structure model includes human Pim-1 kinase amino acid residues 33-305, excluding residues 80-83, of SEQ ID NO:2). Glu79 was built as Ala because electron density was weak for the side chain of this amino acid residue. Ser261 is phosphorylated.

[0024] Figure 2 (2A-1 to 2A-43) lists the atomic structure coordinates in Protein Data Bank (PDB)-like form for phosphorylated Pim-1 in complex with staurosporine (Pim-1-staurosporine complex), as derived by X-ray diffraction from a crystal of the complex. The structure model includes human Pim-1 kinase amino acid residues 33-305, excluding residues 80-83, of SEQ ID NO:2). Glu79 was built as Ala because electron density was weak for the side chain of this amino acid residue. Ser261 is phosphorylated.

[0025] Figure 3 (3A-1 to 3A-43) lists the atomic structure coordinates in Protein Data Bank (PDB)-like form for phosphorylated Pim-1 in complex with LY294002 (Pim-1-LY294002 complex), as derived by X-ray diffraction from a crystal of the complex. The structure model includes human Pim-1 kinase amino acid residues 33-305, excluding residues 80-83, of SEQ ID NO:2). Glu79 was built as Ala because electron density was weak for the side chain of this amino acid residue. Ser261 is phosphorylated.

[0026] Figure 4 depicts a ribbon diagram of the overall fold of the Pim-1–staurosporine complex. The structure is shown with β-strands as arrows and the α-helices as cylinders. The N-terminal domain is in dark grey with an arrow pointing to the glycine rich loop. The hinge connecting the two domains is labeled. The C-terminal domain is shown in light grey with an arrow indicating the activation loop. Staurosporine (represented in stick format) is shown in the active site, bound between Phe49 (glycine rich loop) and the hinge region. The salt bridge stabilizing the conformation of the activation loop is formed by residues Asp200 and Arg166. The site of phosphorylation, Ser261 is shown. All structural figures were prepared with Pymol (DeLano, DeLano Scientific, San Carlos, CA, USA (2002)).

[0027] Figures 5A-5D depict Pim-1, PKA, and PI3K bound to staurosporine, adenosine and ATP. The Pim-1, PKA and PI3K structures were aligned to optimize the superposition of residues adjacent to the hinge regions. In each panel, the Pim-1 structure, carbon, nitrogen, oxygen and other atoms are shown in different shades of grey and amino acid residues are labeled in black type. PKA and PI3K complex structures are drawn in solid color and amino acid residues are labeled in light grey type. Hydrogen bonds are depicted as dotted lines.

[0028] Figure 5A depicts the superposition of PKA-staurosporine complex (Protein Data Bank (PDB) accession number 1STO) and the Pim-1-staurosporine complex. Pim-1 amino acid residues are labeled.

[0029] Figure 5B depicts the superposition of Pim-1-staurosporine and PI3K-staurosporine complexes (PDB accession number 1E8Z). The view is rotated approximately 90° from Figure 4. In this orientation, the glycine-rich loop lies above and in the plane of the page. PI3K amino acid residues are labeled.

[0030] Figure 5C depicts the same overlay as panel B seen from the side to illustrate the relative tilt in the staurosporine ring systems. Pim-1 amino acid residues are labeled.

[0031] Figure 5D depicts the superposition of Pim-1-adenosine and PKA-adenosine complexes (PDB accession number 1FMO). The view is rotated approximately 90° from Figure 4. In this orientation, the glycine-rich loop lies above and in the plane of the page. PKA amino acid residues are labeled.

[0032] Figure 5E depicts the superposition of Pim-1-adenosine and PI3K-ATP complexes (PDB accession number 1E8X). The view is rotated approximately 90° from Figure 4. In this orientation, the glycine-rich loop lies above and in the plane of the page.

[0033] Figure 5F shows a sequence alignment of hinge regions of Pim-1 (amino acid residues 116-132 of SEQ ID NO: 2), amino acid residues 116-131 of PKA (SEQ ID NO: 3), amino acid residues 76-90 of CDK-2 (SEQ ID NO: 4) and amino acid residues 875-891 of PI3K (SEQ ID NO: 5). Residues which accept and donate hydrogen bonds to the adenine ring of ATP are enclosed in boxes.

[0034] Figure 6A depicts the binding site of the Pim-1-LY294002 complex. As drawn, the glycine rich loop would lie above and in the plane of the page. The Fo-Fc electron density map is drawn around the compound at 2.5 sigma level. A water molecule is drawn as a sphere with hydrogen bonds to the chromone oxygen and the Asp186 amide.

[0035] Figure 6B depicts a similar orientation to that in Figure 6A of the binding site of the PI3K-LY294002 complex (PDB accession number 1E7V).

[0036] For Figures 7-9: thick lines connecting atoms (represented as spheres) depict ligand bonds. Thin lines connecting atoms depict non-ligand bonds. Hydrogen bonds are represented by light grey dashed lines. Non-ligand residues involved in hydrophobic contact(s) are depicted by semicircles with lines radiated outwards in the direction of contact. Ligand atoms that are involved in hydrophobic contact(s) are depicted as solid spheres with lines radiating outward in the direction of contact.

[0037] Figure 7 shows a detailed representation of the active site of Pim-1 with adenosine. Hydrogen bonds are shown as dashed lines with the bond length indicated. Atoms and amino acid residues are identified with labels. Molecules labeled A, W and Z are Pim-1 protein, water and adenosine, respectively.

[0038] Figure 8 shows a detailed representation of the active site of Pim-1 with staurosporine. Hydrogen bonds are shown as dashed lines with the bond length indicated. Atoms and amino acid residues are identified with labels. Molecules labeled A, W and Z are Pim-1 protein, water and staurosporine, respectively.

[0039] Figure 9 shows a detailed representation of the active site of Pim-1 with LY294002. Hydrogen bonds are shown as dashed lines with the bond length indicated. Atoms and amino acid residues are identified with labels. Molecules labeled A, W and Z are Pim-1 protein, water and LY294002, respectively.

[0040] Figure 10 shows a diagram of a system used to carry out the instructions encoded by the storage medium of Figures 11 and 12.

[0041] Figure 11 shows a cross section of a magnetic storage medium.

[0042] Figure 12 shows a cross section of a optically-readable data storage medium.

DESCRIPTION OF THE INVENTION

[0043] In order that the invention described herein may be more fully understood, the following detailed description is set forth.

[0044] Throughout the specification, the word "comprise", or variations such as "comprises" or "comprising" will be understood to imply the inclusion of a stated integer or groups of integers but not exclusion of any other integer or groups of integers.

[0045] The following abbreviations are used throughout the application:

A =	Ala =	Alanine	T =	Thr =	Threonine
V =	Val =	Valine	C =	Cys =	Cysteine
L =	Leu =	Leucine	Y =	Tyr =	Tyrosine
I =	Ile =	Isoleucine	N =	Asn =	Asparagine
P =	Pro =	Proline	Q =	Gln =	Glutamine
F =	Phe =	Phenylalanine	D =	Asp =	Aspartic Acid
W =	Trp =	Tryptophan	E =	Glu =	Glutamic Acid
M =	Met =	Methionine	K =	Lys =	Lysine
G =	Gly =	Glycine	R =	Arg =	Arginine
S =	Ser =	Serine	H =	His =	Histidine

Other abbreviations that are used throughout the application include: ADE (for adenosine), STO (for staurosporine), LY2 (for LY294002), PSR (for phosphorylation of Ser261) and CME (for 2-mercaptoethanol modification of Cys161).

[0046] As used herein, the following definitions shall apply unless otherwise indicated.

[0047] The term "about" when used in the context of root mean square deviation (RMSD) values takes into consideration the standard error of the RMSD value, which is ± 0.1 Å.

[0048] The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and a binding pocket or binding site on a protein. The association may be non-covalent -- wherein the juxtaposition is energetically favored by hydrogen bonding, hydrophobic, van der Waals or electrostatic interactions -- or it may be covalent.

[0049] The term "ATP analogue" refers to a compound derived from adenosine-5'-triphosphate (ATP). The compound can be adenosine, AMP, ADP, or a non-hydrolyzable analogue, such as, but not limited to AMP-PNP. The analogue may be in complex with magnesium or manganese ions.

[0050] The term "binding pocket" refers to a region of a molecule or molecular complex, that, as a result of its shape, favorably associates with another chemical entity. The term "pocket" includes, but is not limited to, a cleft, channel or site. Pim-1, Pim-1-like molecules or homologues thereof may have binding pockets which include, but are not limited to, peptide or substrate binding sites, and ATP-binding sites. The shape of a binding pocket may be largely pre-formed before binding of a chemical entity, may be formed simultaneously with binding of a chemical entity, or may be formed by the binding of another chemical entity to a different binding pocket of the molecule, which in turn induces a change in shape of the binding pocket.

[0051] The term "catalytic active site" or "active site" refers to the portion of the protein kinase to which nucleotide substrates bind. For example, the catalytic active site of Pim-1 is at the interface between the N-terminal and C-terminal domains.

[0052] The term "catalytic domain", "kinase catalytic domain", "protein kinase catalytic domain" or "catalytic kinase domain" refers to the kinase domain of a kinase protein. The kinase domain includes the catalytic active site.

[0053] The term "chemical entity" refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes. The chemical entity can be, for example, a ligand, substrate, nucleotide triphosphate, nucleotide diphosphate, phosphate, nucleotide, agonist, antagonist, inhibitor, antibody, peptide, protein or drug. In one embodiment, the chemical entity is an inhibitor or substrate for the active site.

[0054] The term "conservative substitutions" refers to residues that are physically or functionally similar to the corresponding reference residues. That is, a conservative substitution and its reference residue have similar size, shape, electric charge, chemical properties including the ability to form covalent or hydrogen bonds, or the like. Preferred conservative substitutions are those fulfilling the criteria defined for an accepted point mutation in Dayhoff *et al.*, *Atlas of Protein Sequence and Structure* 5: 345-352 (1978 & Supp.), which is incorporated herein by reference. Examples of conservative substitutions are substitutions including but not limited to the following groups: (a) valine, glycine; (b) glycine, alanine; (c) valine, isoleucine, leucine; (d) aspartic acid, glutamic acid; (e) asparagine, glutamine; (f) serine, threonine; (g) lysine, arginine, methionine; and (h) phenylalanine, tyrosine.

[0055] The term "contact score" refers to a measure of shape complementarity between the chemical entity and binding pocket, which is correlated with an RMSD value obtained from a least square superimposition between all or part of the atoms of the chemical entity and all or part of the atoms of the ligand bound (for example, adenosine, staurosporine or LY294002) in the binding pocket according to Figure 1A, 2A or 3A. The docking process may be facilitated by the contact score or RMSD values. For example, if the chemical entity moves to an orientation with high RMSD, the system will resist the motion. A set of orientations of a chemical entity can be ranked by contact score. A lower RMSD value will give a higher contact score. See Meng et al. *J. Comp. Chem.* 4: 505-524 (1992).

[0056] The term "correspond to" or "corresponding amino acid" when used in the context of amino acid residues that correspond to Pim-1 amino acid residues refers to particular amino acid residues or analogues thereof in a Pim-1 protein or homologue thereof that corresponds to amino acid residues in the human Pim-1 protein. The corresponding amino acid may be an identical, mutated, chemically modified, conserved, conservatively substituted, functionally equivalent or homologous amino acid residue when compared to the Pim-1 amino acid residue to which it corresponds. For example, the following are examples of Pim-1 amino acid residues that correspond to PI3K amino acid residues: P125:D884 and V126:A885 (the identity of

the Pim-1 residue is listed first; its position is indicated using Pim-1 sequence numbering; and the identity of PI3K residue is given at the end).

[0057] Methods for identifying a corresponding amino acid are known in the art and are based upon sequence, structural alignment, its functional position, or a combination thereof as compared to the Pim-1 kinase. For example, corresponding amino acids may be identified by superimposing the backbone atoms of the amino acids in Pim-1 and the protein using well known software applications, such as QUANTA (Accelrys, San Diego, CA ©2001, 2002). The corresponding amino acids may also be identified using sequence alignment programs such as the "bestfit" program or CLUSTAL W Alignment Tool (Higgins et al., *Methods Enzymol.* 266: 383-402 (1996)).

[0058] The term "crystallization solution" refers to a solution that promotes crystallization comprising at least one agent, including a buffer, one or more salts, a precipitating agent, one or more detergents, sugars or organic compounds, lanthanide ions, a poly-ionic compound and/or a stabilizer.

[0059] The term "docking" refers to orienting, rotating, translating a chemical entity in the binding pocket, domain, molecule or molecular complex or portion thereof based on distance geometry or energy. Docking may be performed by distance geometry methods that find sets of atoms of a chemical entity that match sets of sphere centers of the binding pocket, domain, molecule or molecular complex or portion thereof. See Meng et al. *J. Comp. Chem.* 4: 505-524 (1992). Sphere centers are generated by providing an extra radius of given length from the atoms (excluding hydrogen atoms) in the binding pocket, domain, molecule or molecular complex or portion thereof. Real-time interaction energy calculations, energy minimizations or rigid-body minimizations (Gschwend et al., *J. Mol. Recognition* 9:175-186 (1996)) can be performed while orienting the chemical entity to facilitate docking. For example, interactive docking experiments can be designed to follow the path of least resistance. If the user in an interactive docking experiment makes a move to increase the energy, the system will resist that move. However, if that user makes a move to decrease energy, the system will favor that move by increased responsiveness. (Cohen et al., *J. Med. Chem.* 33:889-894 (1990)). Docking can also be performed by

combining a Monte Carlo search technique with rapid energy evaluation using molecular affinity potentials. See Goodsell and Olson, *Proteins: Structure, Function and Genetics* 8:195-202 (1990). Software programs that carry out docking functions include but are not limited to MATCHMOL (Cory et al., *J. Mol. Graphics* 2: 39 (1984); MOLFIT (Redington, *Comput. Chem.* 16: 217 (1992)) and DOCK (Meng et al., *supra*).

[0060] The term "generating a three-dimensional structure" or "generating a three-dimensional representation" refers to converting the lists of structure coordinates into structural models or graphical representation in three-dimensional space. This can be achieved through commercially or publicly available software. A model of a three-dimensional structure of a molecule or molecular complex can thus be constructed on a computer screen by a computer that is given the structure coordinates and that comprises the correct software. The three-dimensional structure may be displayed or used to perform computer modeling or fitting operations. In addition, the structure coordinates themselves, without the displayed model, may be used to perform computer-based modeling and fitting operations.

[0061] The term "homologue of Pim-1" or "Pim-1 homologue" refers to a full-length Pim protein other than full-length human Pim-1, or a full-length Pim protein with mutations, conservative substitutions, additions, deletions or a combination thereof, which retains Pim kinase activity. In one embodiment, the additions or deletions are at the N- or C- terminal of the protein, preferrably up to 40, 30, 20 or 10 amino acids. In one embodiment, the homologue is at least 95%, 96%, 97%, 98% or 99% identical in sequence to the full-length Pim-1 protein, and has conservative substitutions as compared to the Pim-1 protein. In one embodiment, the homologue is at least 95%, 96%, 97%, 98% or 99% identical in sequence to amino acid residues 33-305 of SEQ ID NO:2, and has conservative substitutions thereof. Examples of homologues include but are not limited to the following: other human Pim proteins such as human Pim-2, Pim-3 or isoforms thereof, or the foregoing or human Pim-1 with mutations, conservative substitutions, additions, deletions or a combination thereof; or Pim-1, Pim-2, Pim-3 from another species, with mutations, conservative substitutions, additions, deletions or a combination thereof. Such animal species

include, but are not limited to, mouse, rat, a primate such as monkey or other primates.

[0062] The term "homology model" refers to a structural model derived from known three-dimensional structure(s). Generation of the homology model, termed "homology modeling", can include sequence alignment, residue replacement, residue conformation adjustment through energy minimization, or a combination thereof

[0063] The term "interaction energy" refers to the energy determined for the interaction of a chemical entity and a binding pocket, domain, molecule or molecular complex or portion thereof. Interactions include but are not limited to one or more of covalent interactions, non-covalent interactions such as hydrogen bond, electrostatic, hydrophobic, aromatic, van der Waals interactions, and non-complementary electrostatic interactions such as repulsive charge-charge, dipole-dipole and charge-dipole interactions. As interaction energies are measured in negative values, the lower the value the more favorable the interaction.

[0064] The term "motif" refers to a group of amino acid residues in the Pim-1 kinase or homologue that defines a structural compartment or carries out a function in the protein, for example, catalysis, structural stabilization or phosphorylation. The motif may be conserved in sequence, structure and function. The motif can be contiguous in primary sequence or three-dimensional space. Examples of a motif include, but are not limited to, a binding pocket, activation loop, the glycine-rich loop, and the DFG loop (See, Xie et al., *Structure* 6: 983-991 (1998)).

[0065] The term "part of a binding pocket" refers to less than all of the amino acid residues that define the binding pocket. The structure coordinates of amino acid residues that constitute part of a binding pocket may be specific for defining the chemical environment of the binding pocket, or useful in designing fragments of an inhibitor that may interact with those residues. For example, the portion of amino acid residues may be key residues that play a role in ligand binding, or may be residues that are spatially related and define a three-dimensional compartment of the binding pocket. The amino acid residues may be contiguous or non-contiguous in primary sequence. In one embodiment, part of the binding pocket has at least two

amino acid residues, preferably at least three, six, eight, ten, fourteen or fifteen amino acid residues.

[0066] The term "part of a Pim-1 protein" or "part of a Pim-1 homologue" refers to less than all of the amino acid residues of a Pim-1 protein or homologue. In one embodiment, part of the Pim-1 protein or homologue defines the binding pockets, domains, sub-domains, and motifs of the protein or homologue. The structure coordinates of amino acid residues that constitute part of a Pim-1 protein or Pim-1 homologue may be specific for defining the chemical environment of the protein, or useful in designing fragments of an inhibitor that interact with those residues. The portion of amino acid residues may also be residues that are spatially related and define a three-dimensional compartment of the binding pocket, motif or domain. The amino acid residues may be contiguous or non-contiguous in primary sequence. For example, the portion of amino acid residues may be key residues that play a role in ligand or substrate binding, peptide binding, antibody binding, catalysis, structural stabilization or degradation.

[0067] The term "Pim" refers to the kinases from the Pim kinase family. Examples of this family of kinases include but are not limited to Pim-1, Pim-2, Pim-3.

[0068] The term "Pim-1 ATP-binding pocket" refers to a binding pocket of a molecule or molecular complex defined by the structure coordinates of a certain set of amino acid residues present in the Pim-1 structure, as described below. In general, the ligand for the ATP-binding pocket is a nucleotide such as ATP. This binding pocket is in the catalytic active site of the catalytic domain. In the protein kinase family, the ATP-binding pocket is generally located at the interface of the N-terminal and C-terminal domains, and is bordered by the glycine rich loop and the hinge (See, Xie et al., *Structure* 6: 983-991 (1998), incorporated herein by reference).

[0069] The term "Pim-1 inhibitor-binding pocket" refers to that portion of the Pim-1 enzyme active site to which the inhibitor binds. The inhibitor-binding pocket is defined by the structure coordinates of a certain set of amino acid residues present in the Pim-1-inhibitor structure, as described below.

[0070] The term "Pim-1-like" refers to all or a portion of a molecule or molecular complex that has a commonality of shape to all or a portion of the Pim-1 protein. For example, in the Pim-1-like inhibitor-binding pocket, the commonality of shape is defined by a root mean square deviation of the structure coordinates of the backbone atoms between the amino acids in the Pim-1-like inhibitor-binding pocket and the Pim-1 amino acids in the Pim-1 inhibitor-binding pocket as set forth in Figures 1A, 2A and 3A. Compared to the amino acids of the Pim-1 inhibitor-binding pocket, the corresponding amino acid residues in the Pim-1-like binding pocket may or may not be identical. Depending on the set of Pim-1 amino acid residues that define the Pim-1 inhibitor-binding pocket, one skilled in the art would be able to locate the corresponding amino acid residues that define a Pim-1-like binding pocket in a protein based on sequence or structural homology.

[0071] The term "Pim-1 protein" or "full-length Pim-1 protein" refers to human Pim-1 protein (amino acid residues 1 to 313; SwissProt entry P11309; SEQ ID NO:2).

[0072] The term "Pim-1 protein complex" or "Pim-1 homologue complex" refers to a molecular complex formed by associating the Pim-1 protein or Pim-1 homologue with a chemical entity, for example, a ligand, a substrate, nucleotide triphosphate, nucleotide diphosphate, phosphate, an agonist or antagonist, inhibitor, antibody, drug or compound.

[0073] The term "protein complex", "complex" or "molecular complex" refers to a protein or section of a protein associated with a chemical entity.

[0074] The term "quantified association" refers to calculations of distance geometry and energy. Energy can include but is not limited to interaction energy, free energy and deformation energy. See Cohen, *supra*.

[0075] The term "root mean square deviation" or "RMSD" means the square root of the arithmetic mean of the squares of the deviations from the mean. It is a way to express the deviation or variation from a trend or object. For purposes of the invention, the "root mean square deviation" defines the variation in the backbone atoms of Pim-1, a binding pocket, a motif, a domain, or portion thereof, as defined by

the structure coordinates of Pim-1 described herein. It would be apparent to the skilled worker that the calculation of RMSD involves a standard error of ± 0.1 Å.

[0076] The term "soaked" refers to a process in which the crystal is transferred to a solution containing the compound of interest.

[0077] The term "structure coordinates" refers to Cartesian coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a protein or protein complex in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are then used to establish the positions of the individual atoms of the molecule or molecular complex.

[0078] The term "sub-domain" refers to a portion of the domain.

[0079] The term "substantially all of a Pim-1 binding pocket" or "substantially all of a Pim-1 protein" refers to all or almost all of the amino acids in the Pim-1 binding pocket or protein. For example, substantially all of a Pim-1 binding pocket can be 100%, 95%, 90%, 80%, or 70% of the residues defining the Pim-1 binding pocket or protein.

[0080] The term "substrate binding pocket" refers to the binding pocket for a substrate of Pim-1 or homologue thereof. A substrate is generally defined as the molecule upon which an enzyme performs catalysis. Natural substrates, synthetic substrates or peptides, or mimics of a natural substrates of Pim-1 or homologue thereof may associate with the substrate binding pocket.

[0081] The term "sufficiently homologous to Pim-1" refers to a protein that has a sequence identity of at least 25% compared to Pim-1 protein. In other embodiments, the sequence identity is at least 40%. In other embodiments, the sequence identity is at least 50%, 60%, 70%, 80%, 90%, 95%, 96%, 97%, 98% or 99%.

[0082] The term "three-dimensional structural information" refers to information obtained from the structure coordinates. Structural information generated can include the three-dimensional structure or graphical representation of the structure. Structural

information can also be generated when subtracting distances between atoms in the structure coordinates, calculating chemical energies for a Pim-1 molecule or molecular complex or homologues thereof, calculating or minimizing energies for an association of a Pim-1 molecule or molecular complex or homologues thereof to a chemical entity.

Crystallizable Compositions and Crystals of Pim-1 Protein and Complexes Thereof

[0083] According to one embodiment, the invention provides a crystal or crystallizable composition comprising Pim-1 protein, Pim-1 protein complex or homologues thereof. In one embodiment, the Pim-1 protein or homologue is phosphorylated. In another embodiment, the chemical entity is an ATP analogue, nucleotide triphosphate, nucleotide diphosphate, phosphate, adenosine, stauropsorine, LY294002, or active site inhibitor. In one embodiment the chemical entity is adenosine, staurosporine or LY294002.

[0084] The Pim-1 protein homologue in the crystal may be a truncated Pim-1 protein comprising amino acid residues 33 to 305 of SEQ ID NO:2, or full length or truncated Pim-1 protein with conservative substitutions.

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         10         20         30         40         50
MLLSKINSLA HLRAAPCNDL HATKLAPGKE KEPLESQYQV GPLLGSGGFG
         60         70         80         90        100
SVYSGIRVSD NLPVAIKHVE KDRISDWGEL PNGTRVPMEV VLLKKVSSGF
        110        120        130        140        150
SGVIRLLDWF ERPDSFVLIL ERPEPVQDLF DFITERGALQ EELARSFFWQ
        160        170        180        190        200
VLEAVRHCHN CGVLHRDIKD ENILIDLNRG ELKLIDFGSG ALLKDTVYTD
        210        220        230        240        250
FDGTRVYSPP EWIRYHRYHG RSAAVWSLGI LLYDMVCGDI PFEHDEEIIR
        260        270        280        290        300
GQVFFRQRVS SECQHLIRWC LALRPSDRPT FEEIQNHPWM QDVLLPQETA
        310
EIHLHSLSPG PSK          SEQ ID NO:2 (SwissProt entry P11309)
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[0085] The crystallizable compositions may further comprise a crystallization solution of 0.025 to 1.5 M $(NH_4)_2HPO_4$, 0-200 mM citrate buffer at pH 4.0 and 7.5, and 0-300 mM NaCl. In one embodiment, the crystallizable compositions comprise a crystallization solution of equal volumes of Pim-1 protein (12 mg/ml protein in 20 mM HEPES at pH 8, 100 mM NaCl and 5 mM DTT) and a solution of 1.0 M $(NH_4)_2HPO_4$, 100 mM citrate buffer at pH 5.5, and 100 mM NaCl.

[0086] According to one embodiment, the invention provides for a crystal with unit cell dimensions of a= 98.27 Å b= 98.27 Å, c= 80.39 Å, $\alpha = \beta = 90$, $\gamma = 120°$ and space group $P6_5$. Preferably, the crystal comprises the Pim-1-adenosine complex.

[0087] In another embodiment, the invention provides for a crystal with unit cell dimensions a= 97.73 Å b= 97.73 Å, c= 80.51 Å, $\alpha = \beta = 90$, $\gamma = 120°$ and space group $P6_5$. Preferably, the crystal comprises the Pim-1-staurosporine complex.

[0088] According to another embodiment, the invention provides for a crystal with unit cell dimensions a= 97.65 Å b= 97.65 Å, c= 80.72 Å, $\alpha = \beta = 90$, $\gamma = 120°$ and space group $P6_5$. Preferably, the crystal comprises the Pim-1-LY294002 complex.

[0089] It will be readily apparent to those skilled in the art that the unit cells of the crystal compositions may deviate up to ± 1-2 Å from the above cell dimensions depending on the deviation in the unit cell calculations or conformational change in the protein.

[0090] The Pim-1 protein or homologue thereof may be produced by any well-known method, including synthetic methods, such as solid phase, liquid phase and combination solid phase/liquid phase syntheses; recombinant DNA methods, including cDNA cloning, optionally combined with site directed mutagenesis; and/or purification of the natural products. In one embodiment, the protein is overexpressed from an *E. coli* system.

Methods of Obtaining Crystals of Pim-1 Protein, Complexes Thereof or Homologues Thereof

[0091] The invention also relates to a method of obtaining a crystal of Pim-1 protein or Pim-1 homologue thereof, comprising the steps of:

a) producing and purifying a Pim-1 protein or homologue thereof;

b) combining a crystallizable solution with said Pim-1 protein or homologue thereof to produce a crystallizable composition; and

c) subjecting said crystallizable composition to conditions which promote crystallization and obtaining said crystals.

[0092] The invention also relates to a method of obtaining a crystal of a Pim-1 protein complex or Pim-1 homologue complex, further comprising the step of:

d) soaking said crystal in a buffer solution comprising a chemical entity.

[0093] The invention also relates to a method of obtaining a crystal of a Pim-1 protein complex or Pim-1 homologue complex, comprising the steps of:

a) producing and purifying a Pim-1 protein or homologue thereof;

b) combining a crystallizable solution with said Pim-1 protein or homologue thereof in the presence of a chemical entity to produce a crystallizable composition; and

c) subjecting said crystallizable composition to conditions which promote crystallization and obtaining said crystals.

[0094] In one embodiment, the chemical entity is selected from the group consisting of an ATP analogue, nucleotide triphosphate, nucleotide diphosphate, phosphate, adenosine, staurosporine, substrate inhibitor, or active site inhibitor. In another embodiment, the crystallization solution is as described previously. In another embodiment, the crystallizable composition is treated with micro-crystals of Pim-1 or Pim-1 complexes or homologues thereof.

[0095] In certain embodiments, the method of making crystals of Pim-1 protein complexes or homologues thereof includes the use of a device for promoting crystallizations. Devices for promoting crystallization can include but are not limited to the hanging-drop, sitting-drop, dialysis or microtube batch devices. (U.S. patent 4,886,646, 5,096,676, 5,130,105, 5,221,410 and 5,400,741; Pav *et al.*, *Proteins: Structure, Function, and Genetics* 20: 98-102 (1994), incorporated herein by reference). The hanging-drop, sitting-drop, and some adaptations of the microbatch methods (D'Arcy et al., *J. Cryst. Growth* 168: 175-180 (1996) and Chayen, *J. Appl. Cryst.* 30: 198-202 (1997)) produce crystals by vapor diffusion. The hanging drop and sitting drop containing the crystallizable composition is equilibrated in a reservoir containing a higher or lower concentration of the precipitant. As the drop approaches equilibrium with the reservoir, the saturation of protein in the solution leads to the formation of crystals.

[0096] Microseeding or seeding may be used to increase the size and quality of crystals. In this instance, micro-crystals are crushed to yield a stock seed solution. The stock seed solution is diluted in series. Using a needle, glass rod, micro-pipet, micro-loop or strand of hair, a small sample from each diluted solution is added to a set of equilibrated drops containing a protein concentration equal to or less than a concentration needed to create crystals without the presence of seeds. The aim is to end up with a single seed crystal that will act to nucleate crystal growth in the drop.

[0097] It would be readily apparent to one of skill in the art to vary the crystallization conditions disclosed above to identify other crystallization conditions that would produce crystals of Pim-1 homologue, Pim-1 homologue complex, Pim-1 protein or other Pim-1 protein complexes. Such variations include, but are not limited to, adjusting pH, protein concentration and/or crystallization temperature, changing the identity or concentration of salt and/or precipitant used, using a different method of crystallization, or introducing additives such as detergents (e.g., TWEEN 20 (monolaurate), LDAO, Brij 30 (4 lauryl ether)), sugars (e.g., glucose, maltose), organic compounds (e.g., dioxane, dimethylformamide), lanthanide ions or polyionic compounds that aid in crystallization. High throughput crystallization assays may also be used to assist in finding or optimizing the crystallization condition.

Binding Pockets of Pim-1 Protein or Homologues Thereof

[0098] As disclosed herein, applicants have provided the three-dimensional X-ray structures of Pim-1-adenosine, Pim-1-staurosporine and Pim-1-LY294002 complexes. The atomic coordinates for the structures of Pim-1-adenosine, Pim-1-staurosporine and Pim-1-LY294002 complexes are presented in Figures 1A, 2A and 3A, respectively.

[0099] To use the structure coordinates generated for the Pim-1 complexes or one of their binding pockets or homologues thereof, it may be necessary to convert the structure coordinates, or portions thereof, into a three-dimensional shape (i.e., a three-dimensional representation of these complexes or binding pockets). This is achieved through the use of a computer and commercially available software that is capable of generating the three-dimensional representations or structures of molecules or molecular complexes, or portions thereof, from a set of structural coordinates. These three-dimensional representations may be displayed on a computer screen.

[0100] Binding pockets, also referred to as binding sites in the present invention, are of significant utility in fields such as drug discovery. The association of natural ligands or substrates with the binding pockets of their corresponding receptors or enzymes is the basis of many biological mechanisms of action. Similarly, many drugs exert their biological effects through association with the binding pockets of receptors and enzymes. Such associations may occur with all or part of the binding pocket. An understanding of such associations will help lead to the design of drugs having more favorable associations with their target receptor or enzyme, and thus, improved biological effects. Therefore, this information is valuable in designing potential inhibitors of the binding pockets of biologically important targets. The binding pockets of this invention will be important for drug design.

[0101] The conformations of Pim-1 and other proteins at a particular amino acid site, along the polypeptide backbone, can be compared using well-known procedures for performing sequence alignments of the amino acids. Such sequence alignments allow for the equivalent sites on these proteins to be compared. Such methods for performing sequence alignment include, but are not limited to, the "bestfit" program and CLUSTAL W Alignment Tool, Higgins et al., *supra.*

[0102] Figures 5, 6 and 7 show a detailed representation of the active sites of Pim-1-adenosine, Pim-1-staurosporine and Pim-1-LY294002 complexes, respectively. Pim-1 amino acids Phe49, Ala65, Glu121, Arg122, Asp128, and Leu174 form an inhibitor-binding pocket through their contacts with adenosine in the Pim-1-adenosine complex (Figure 7). Pim-1 amino acids Leu44, Gly45, Phe49, Val52, Ala65, Lys67, Ile104, Leu120, Glu121, Val126, Asp128, Glu171, Leu174, Ile185 and Asp186 form an inhibitor-binding pocket through their contacts with staurosporine in the Pim-1-staurosporine complex (Figure 8). Pim-1 amino acids Leu44, Gly45, Phe49, Val52, Ala65, Lys67, Ile104, Leu120, Arg122, Val126, Leu174 and Asp 186 form an inhibitor-binding pocket through their contacts with LY294002 in the Pim-1-LY294002 complex (Figure 9). Asp186 makes a water-mediated contact in the Pim-1-LY294002 complex. Pim-1 amino acid residues Phe49, Ala65 and Leu174 are found to contact the inhibitors in all three complex structures in Figure 1A, 2A or 3A.

[0103] Pro123 and Val126 are residues unique to Pim-1 as discussed in Example 8. Accordingly, in one embodiment, an inhibitor-binding pocket comprises Pim-1 amino acid residues Phe49, Ala65, Pro123, Val 126 and Leu174 according to the structure of Pim-1 protein in Figure 1A, 2A or 3A. In another embodiment, an inhibitor-binding pocket comprises Pim-1 amino acid residues Phe49, Ala65, Val 126 and Leu174 according to the structure of Pim-1 protein in Figure 1A, 2A or 3A.

[0104] In another embodiment, the inhibitor-binding pocket comprises amino acid residues Leu44, Gly45, Phe49, Val52, Ala65, Ile104, Leu120, Glu121, Arg122, Pro123, Val126, Asp128, Asp131, Glu171, Leu174, and Ile185 according to the structure of the Pim-1-adenosine complex in Figure 1A. In another embodiment, the inhibitor-binding pocket comprises amino acid residues Leu44, Gly45, Ser46, Phe49, Val52, Ala65, Lys67, Glu89, Ile104, Leu120, Glu121, Arg122, Pro123, Val126, Asp128, Glu171, Asn172, Leu174, Ile185 and Asp186 according to the structure of the Pim-staurosporine complex in Figure 2A. In another embodiment, the inhibitor-binding pocket comprises amino acid residues Leu44, Gly45, Ser46, Phe49, Val52, Ala65, Lys67, Ile104, Leu120, Glu121, Arg122, Val126, Leu174, Ile185 and Asp186 according to the structure of Pim-1-LY294002 in Figure 3A. These amino acid residues are within 5 Å ("5 Å sphere of amino acids") of adenosine, staurosporine or

LY294002 bound in the inhibitor-binding pockets as identified using the program Swiss-Pdb Viewer (Guex, N. and Peitsch, M.C. (1997) "SWISS-MODEL and the Swiss-PdbViewer: An environment for comparative protein modeling", *Electrophoresis* 18: 2714-2723).

[0105] In one embodiment, the inhibitor-binding pocket comprises amino acid residues Leu44, Gly45, Phe49, Val52, Ala65, Ile104, Leu120, Glu121, Arg122, Val126, Leu174, and Ile185 according to the structure of the Pim-1-inhibitor complex in Figure 1A, 2A or 3A. These are the common amino acid residues within 5 Å of the inhibitor in the three complex structures.

[0106] In another embodiment, the inhibitor-binding pocket comprises amino acid residues Leu43, Leu44, Gly45, Ser46, Gly47, Phe49, Gly50, Ser51, Val52, Tyr53, Ser54, Pro63, Val64, Ala65, Ile66, Lys67, Val103, Ile104, Arg105, Leu118, Ile119, Leu120, Glu121, Arg122, Pro123, Glu124, Val126, Gln127, Asp128, Leu129, Phe130, Asp131, Lys169, Asp170, Glu171, Asn172, Ile173, Leu174, Ile175, Lys183, Leu184, Ile185 and Asp186 according to the structure of the Pim-1-adenosine complex in Figure 1A. In another embodiment, the inhibitor-binding pocket comprises amino acid residues Leu43, Leu44, Gly45, Ser46, Gly47, Gly48, Phe49, Gly50, Ser51, Val52, Tyr53, Ser54, Pro63, Val64, Ala65, Ile66, Lys67, Val69, Glu89, Leu93, Ile104, Arg105, Leu118, Ile119, Leu120, Glu121, Arg122, Pro123, Glu124, Pro125, Val126, Gln127, Asp128, Leu129, Phe130, Asp131, Asp167, Lys169, Asp170, Glu171, Asn172, Ile173, Leu174, Ile175, Lys183, Leu184, Ile185, Asp186, Phe187 and Gly188 according to the structure of the Pim-staurosporine complex in Figure 2A. In another embodiment, the inhibitor-binding pocket comprises amino acid residues Leu43, Leu44, Gly45, Ser46, Gly47, Gly48, Phe49, Gly50, Ser51, Val52, Tyr53, Ser54, Gly55, Val64, Ala65, Ile66, Lys67, Glu89, Leu93, Val103, Ile104, Arg105, Leu118, Ile119, Leu120, Glu121, Arg122, Pro123, Glu124, Pro125, Val126, Gln127, Asp128, Asp131, Glu171, Asn172, Ile173, Leu174, Ile175, Lys183, Leu184, Ile185, Asp186, Phe187 and Gly188 according to the structure of Pim-1-LY294002 in Figure 3A. These amino acid residues are within 8 Å ("8 Å sphere of amino acids") of adenosine, staurosporine or LY294002 bound in the inhibitor-binding pockets as identified using the program Swiss-Pdb Viewer (Guex, N. and

Peitsch, M.C. (1997) "SWISS-MODEL and the Swiss-PdbViewer: An environment for comparative protein modeling", *Electrophoresis* 18: 2714-2723).

[0107] In one embodiment, the inhibitor-binding pocket comprises amino acid residues Leu43, Leu44, Gly45, Ser46, Gly47, Phe49, Gly50, Ser51, Val52, Tyr53, Ser54, Val64, Ala65, Ile66, Lys67, Ile104, Arg105, Leu118, Ile119, Leu120, Glu121, Arg122, Pro123, Glu124, Val126, Gln127, Asp128, Asp131, Glu171, Asn172, Ile173, Leu174, Ile175, Lys183, Leu184, Ile185 and Asp186 according to the structure of Pim-1-inhibitor complex in Figure 1A, 2A or 3A. These are the common amino acid residues within 8 Å of the inhibitor in the three complex structures.

[0108] It will be readily apparent to those of skill in the art that the numbering of amino acid residues in homologues of human Pim-1 may be different than that set forth for human Pim-1. Corresponding amino acids in Pim-1 homologues are easily identified by visual inspection of the amino acid sequences or by using commercially available homology software programs. Homologues of Pim-1 include, for example, Pim-1 from other species, such as non-humans primates, mouse, rat, etc.

[0109] Those of skill in the art understand that a set of structure coordinates for an enzyme or an enzyme-complex, or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations in the individual coordinates will have little effect on overall shape. In terms of binding pockets, these variations would not be expected to significantly alter the nature of ligands that could associate with those pockets.

[0110] The variations in coordinates discussed above may be generated because of mathematical manipulations of the Pim-1-adenosine structure coordinates. For example, the structure coordinates set forth in Figure 1A, 2A or 3A may undergo crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above.

[0111] Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of

the components that make up the crystal may also account for variations in structure coordinates. If such variations are within a certain root mean square deviation as compared to the original coordinates, the resulting three-dimensional shape is considered encompassed by this invention. Thus, for example, a ligand that bound to the inhibitor-binding pocket of Pim-1 would also be expected to bind to another binding pocket whose structure coordinates defined a shape that fell within the RMSD value.

[0112] Various computational analyses may be necessary to determine whether a molecule or binding pocket, or portion thereof, is sufficiently similar to the binding pockets above-described. Such analyses may be carried out in well known software applications, such as ProFit (A. C.R. Martin, ProFit version 1.8, http://www.bioinf.org.uk/software), Swiss-Pdb Viewer (Guex et al., *Electrophoresis* 18: 2714-2723 (1997)), the Molecular Similarity application of QUANTA (Accelrys, San Diego, CA © 2001, 2002) and as described in the accompanying User's Guide, which are incorporated herein by reference.

[0113] The above programs permit comparisons between different structures, different conformations of the same structure, and different parts of the same structure. The procedure used in QUANTA (Accelrys, San Diego, CA ©2001, 2002) and Swiss-Pdb Viewer (Guex and Peitsch, *Electrophoresis* 18: 2714-2723 (1997) to compare structures is divided into four steps: 1) load the structures to be compared; 2) define the atom equivalences in these structures; 3) perform a fitting operation on the structures; and 4) analyze the results.

[0114] The procedure used in ProFit to compare structures includes the following steps: 1) load the structures to be compared; 2) specify selected residues of interest; 3) define the atom equivalences in the selected residues; 4) perform a fitting operation on the selected residues; and 5) analyze the results.

[0115] Each structure in the comparison is identified by a name. One structure is identified as the target (i.e., the fixed structure); all remaining structures are working structures (i.e., moving structures). Since atom equivalency within QUANTA (Accelrys, San Diego, CA ©2001, 2002) is defined by user input, for the purposes of this invention, we will define equivalent atoms as protein backbone atoms N, O, C

and Cα for all corresponding amino acid residues between two structures being compared.

[0116] The corresponding amino acids may be identified by sequence alignment programs such as the "bestfit" program available from the Genetics Computer Group which uses the local homology algorithm described by Smith and Waterman in *Advances in Applied Mathematics* 2: 482 (1981), which is incorporated herein by reference. A suitable amino acid sequence alignment will require that the proteins being aligned share minimum percentage of identical amino acids. Generally, a first protein being aligned with a second protein should share in excess of about 35% identical amino acids (Hanks et al., *Science* 241: 42 (1988); Hanks and Quinn, *Methods in Enzymology* 200: 38 (1991)). The identification of equivalent residues can also be assisted by secondary structure alignment, for example, aligning the α-helices, β-sheets in the structure. The program Swiss-Pdb viewer (Guex and Peitsch, *Electrophoresis* 18: 2714-2723 (1997) utilizes a best fit algorithm that is based on secondary sequence alignment.

[0117] When a rigid fitting method is used, the working structure is translated and rotated to obtain an optimum fit with the target structure. The fitting operation uses an algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in angstroms, is reported by the above programs. The Swiss-Pdb Viewer (Guex and Peitsch, *Electrophoresis* 18: 2714-2723 (1997) program sets an RMSD cutoff for eliminating pairs of equivalent atoms that have high RMSD values. An RMSD cutoff value can be used to exclude pairs of equivalent atoms with extreme individual RMSD values. In the program ProFit, the RMSD cutoff value can be specified by the user.

[0118] For the purpose of this invention, any molecule, molecular complex, binding pocket, motif, domain thereof or portion thereof that is within a root mean square deviation for backbone atoms (N, Cα, C, O) when superimposed on the relevant backbone atoms described by structure coordinates listed in Figure 1A, 2A or 3A are encompassed by this invention.

[0119] The RMSD values of all backbone atoms between Pim-1-adenosine and Pim-1-staurosporine complexes, and Pim-1-LY294002 complex were 0.47 Å and 0.31 Å, respectively. RMSD values of the binding pockets comprising amino acid residues Leu43, Leu44, Gly45, Ser46, Gly47, Phe49, Gly50, Ser51, Val52, Tyr53, Ser54, Val64, Ala65, Ile66, Lys67, Ile104, Arg105, Leu118, Ile119, Leu120, Glu121, Arg122, Pro123, Glu124, Val126, Gln127, Asp128, Asp131, Glu171, Asn172, Ile173, Leu174, Ile175, Lys183, Leu184, Ile185 and Asp186 in the Pim-1-adenosine and Pim-1-staurosporine complexes, and Pim-1-LY294002 complex were 0.44 Å and 0.37 Å, respectively. The RMSD values between the binding pockets comprising amino acid residues Leu44, Gly45, Phe49, Val52, Ala65, Lys67, Ile104, Leu120, Arg122, Val126, and Leu174 Asp186 in the Pim-1-adenosine and Pim-1-staurosporine complexes, and the Pim-1-LY294002 complex were 0.48 Å and 0.42 Å, respectively. The RMSD values between the binding pockets comprising amino acid residues Phe49, Ala65, Val126, and Asp186 in the Pim-1-adenosine and Pim-1-staurosporine complexes, and the Pim-1-LY294002 complex were 0.61 Å and 0.55 Å, respectively. All RMSD values were calculated by comparing the backbone atoms (N, Cα, C, O) of structures.

[0120] One embodiment of this invention provides a crystalline molecule or molecular complex comprising a protein defined by structure coordinates of a set of amino acid residues that are identical to Pim-1 amino acid residues according to Figure 1A, 2A or 3A, wherein the RMSD between said set of amino acid residues and said human Pim-1 kinase amino acid residues is not more than about 3.0 Å. In other embodiments, the RMSD between said set of amino acid residues and said human Pim-1 kinase amino acid residues is not greater than about 2.0 Å, not greater than about 1.0 Å, or not greater than about 0.5 Å.

[0121] In one embodiment, the present invention provides a crystalline molecule or molecular complex comprising all or part of a binding pocket defined by a set of amino acid residues which are identical to human Pim-1 kinase amino acid residues Leu43, Leu44, Gly45, Ser46, Gly47, Phe49, Gly50, Ser51, Val52, Tyr53, Ser54, Val64, Ala65, Ile66, Lys67, Ile104, Arg105, Leu118, Ile119, Leu120, Glu121, Arg122, Pro123, Glu124, Val126, Gln127, Asp128, Asp131, Glu171, Asn172, Ile173,

Leu174, Ile175, Lys183, Leu184, Ile185 and Asp186 according to Figure 1A, 2A or 3A, wherein the RMSD of the backbone atoms between said human Pim-1 kinase amino acid residues and said amino acid residues which are identical is not greater than about 2.0 Å. In other embodiments, the RMSD is not greater than about 1.5 Å, 1.0 Å, 0.8 Å, 0.5 Å, 0.3 Å, or 0.2 Å. In other embodiments, the binding pocket is defined by a set of amino acid residues comprising at least twelve, fourteen, sixteen, eighteen, nineteen, twenty-one, twenty-three or twenty-five amino acid residues which are identical to said human Pim-1 kinase amino acid residues.

[0122] In one embodiment, the present invention provides a crystalline molecule or molecular complex comprising all or part of a binding pocket defined by a set of amino acid residues which are identical to human Pim-1 kinase amino acid residues Leu44, Gly45, Phe49, Val52, Ala65, Lys67, Ile104, Leu120, Arg122, Val126, and Leu174 according to Figure 3A, wherein the RMSD of the backbone atoms between said human Pim-1 kinase amino acid residues and said set of amino acid residues which are identical is not greater than about 2.0 Å. In other embodiments, the RMSD is not greater than about 1.5 Å, 1.0 Å, 0.8Å, 0.5 Å, 0.3 Å, or 0.2 Å. In other embodiments, the binding pocket is defined by a set of amino acid residues comprising at least eight, nine, ten or eleven amino acid residues which are identical to said human Pim-1 kinase amino acid residues.

[0123] In one embodiment, the present invention provides a crystalline molecule or molecular complex comprising all or part of a binding pocket defined by a set of amino acid residues which are identical to human Pim-1 kinase amino acid residues Phe49, Ala65, Val126, and Leu174 according to Figure 1A, 2A or 3A, wherein the RMSD of the backbone atoms between said human Pim-1 kinase amino acid residues and said set of amino acid residues which are identical is not greater than about 2.0 Å. In other embodiments, the RMSD is not greater than about 1.5 Å, 1.0 Å, 0.8 Å, 0.5 Å, 0.3 Å, or 0.2 Å.

Computer Systems

[0124] According to another embodiment, this invention provides a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines the above-mentioned molecules or molecular complexes. In one embodiment, the data defines the above-mentioned binding pockets by comprising the structure coordinates of said amino acid residues according to Figure 1A, 2A or 3A. To use the structure coordinates generated for Pim-1, homologues thereof, or one of its binding pockets, it is at times necessary to convert them into a three-dimensional shape or to extract three-dimensional structural information from them. This is achieved through the use of commercially or publicly available software that is capable of generating a three-dimensional structure or a three-dimensional representation of molecules or portions thereof from a set of structure coordinates. In one embodiment, three-dimensional structure or representation may be displayed graphically.

[0125] Therefore, according to another embodiment, this invention provides a machine-readable data storage medium comprising a data storage material encoded with machine readable data. In one embodiment, a machine programmed with instructions for using said data is capable of generating a three-dimensional structure or three-dimensional representation of any of the molecules, or molecular complexes or binding pockets thereof, that are described herein.

[0126] This invention also provides a computer comprising:

(a) a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines any one of the above molecules or molecular complexes;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central processing unit (CPU) coupled to said working memory and to said machine-readable data storage medium for processing said

machine readable data and means for generating three-dimensional structural information of said molecule or molecular complex; and

(d) output hardware coupled to said central processing unit for outputting three-dimensional structural information of said molecule or molecular complex, or information produced by using said three-dimensional structural information of said molecule or molecular complex.

[0127] In one embodiment, the data defines the binding pocket of the molecule or molecular complex.

[0128] Three-dimensional data generation may be provided by an instruction or set of instructions such as a computer program or commands for generating a three-dimensional structure or graphical representation from structure coordinates, or by subtracting distances between atoms, calculating chemical energies for a Pim-1 molecule or molecular complex or homologues thereof, or calculating or minimizing energies for an association of a Pim-1 molecule or molecular complex or homologues thereof to a chemical entity. The graphical representation can be generated or displayed by commercially available software programs. Examples of software programs include but are not limited to QUANTA (Accelrys, San Diego, CA ©2001, 2002), O (Jones *et al.*, *Acta Crystallogr.* A47: 110-119 (1991)) and RIBBONS (Carson, *J. Appl. Crystallogr.* 24: 958-961 (1991)), which are incorporated herein by reference. Certain software programs may imbue this representation with physico-chemical attributes which are known from the chemical composition of the molecule, such as residue charge, hydrophobicity, torsional and rotational degrees of freedom for the residue or segment, etc. Examples of software programs for calculating chemical energies are described in the Rational Drug Design section.

[0129] Information of said binding pocket or information produced by using said binding pocket can be outputted through display terminals, touchscreens, facsimile machines, modems, CD-ROMs, printers, a CD or DVD recorder, ZIP™ or JAZ™ drives or disk drives. The information can be in graphical or alphanumeric form.

[0130] In one embodiment, the computer is executing an instruction such as a computer program for generating three-dimensional structure or docking. In another embodiment, the computer further comprises a commercially available software program to display the information as a graphical representation. Examples of software programs include but as not limited to, QUANTA (Accelrys, San Diego, CA ©2001, 2002), O (Jones *et al.*, *Acta Crystallogr.* A47: 110-119 (1991)) and RIBBONS (Carson, *J. Appl. Crystallogr.* 24: 958-961 (1991)), all of which are incorporated herein by reference.

[0131] Figure 10 demonstrates one version of these embodiments. System (10) includes a computer (11) comprising a central processing unit ("CPU") (20), a working memory (22) which may be, e.g., RAM (random-access memory) or "core" memory, mass storage memory (24) (such as one or more disk drives, CD-ROM drives or DVD-ROM drives), one or more cathode-ray tube ("CRT") display terminals (26), one or more keyboards (28), one or more input lines (30), and one or more output lines (40), all of which are, interconnected by a conventional bi-directional system bus (50).

[0132] Input hardware (35), coupled to computer (11) by input lines (30), may be implemented in a variety of ways. Machine-readable data of this invention may be inputted via the use of a modem or modems (32) connected by a telephone line or dedicated data line (34). Alternatively or additionally, the input hardware (35) may comprise CD-ROM or DVD-ROM drives or disk drives (24). In conjunction with display terminal (26), keyboard (28) may also be used as an input device.

[0133] Output hardware (46), coupled to computer (11) by output lines (40), may similarly be implemented by conventional devices. By way of example, output hardware (46) may include CRT display terminal (26) for displaying a graphical representation of a binding pocket of this invention using a program such as QUANTA (Accelrys, San Diego, CA ©2001, 2002) as described herein. Output hardware may also include a printer (42), so that hard copy output may be produced, or a disk drive (24), to store system output for later use. Output hardware may also include a display terminal, touchscreens, facsimile machines, modems, a CD or DVD

recorder, ZIP™ or JAZ™ drives, disk drives, or other machine-readable data storage device.

[0134] In operation, CPU (20) coordinates the use of the various input and output devices (35), (46), coordinates data accesses from mass storage (24) and accesses to and from working memory (22), and determines the sequence of data processing steps. A number of programs may be used to process the machine-readable data of this invention. Such programs are discussed in reference to the computational methods of drug discovery as described herein. Specific references to components of the hardware system (10) are included as appropriate throughout the following description of the data storage medium.

[0135] Figure 11 shows a cross section of a magnetic data storage medium (100) which can be encoded with a machine-readable data that can be carried out by a system such as system (10) of Figure 10. Medium (100) can be a conventional floppy diskette or hard disk, having a suitable substrate (101), which may be conventional, and a suitable coating (102), which may be conventional, on one or both sides, containing magnetic domains (not visible) whose polarity or orientation can be altered magnetically. Medium (100) may also have an opening (not shown) for receiving the spindle of a disk drive or other data storage device (24).

[0136] The magnetic domains of coating (102) of medium (100) are polarized or oriented so as to encode in manner which may be conventional, machine readable data such as that described herein, for execution by a system such as system (10) of Figure 10.

[0137] Figure 12 shows a cross section of an optically-readable data storage medium (110) which also can be encoded with such a machine-readable data, or set of instructions, which can be carried out by a system such as system (10) of Figure 10. Medium (110) can be a conventional compact disk read only memory (CD-ROM) or a rewritable medium such as a magneto-optical disk which is optically readable and magneto-optically writable. Medium (100) preferably has a suitable substrate (111),

which may be conventional, and a suitable coating (112), which may be conventional, usually of one side of substrate (111).

[0138] In the case of CD-ROM, as is well known, coating (112) is reflective and is impressed with a plurality of pits (113) to encode the machine-readable data. The arrangement of pits is read by reflecting laser light off the surface of coating (112). A protective coating (114), which preferably is substantially transparent, is provided on top of coating (112).

[0139] In the case of a magneto-optical disk, as is well known, coating (112) has no pits (113), but has a plurality of magnetic domains whose polarity or orientation can be changed magnetically when heated above a certain temperature, as by a laser (not shown). The orientation of the domains can be read by measuring the polarization of laser light reflected from coating (112). The arrangement of the domains encodes the data as described above.

[0140] In one embodiment, the structure coordinates of said molecules or molecular complexes are produced by homology modeling of at least a portion of the structure coordinates of Figures 1A, 2A or 3A. Homology modeling can be used to generate structural models of Pim-1 homologues or other homologous proteins based on the known structure of Pim-1. This can be achieved by performing one or more of the following steps: performing sequence alignment between the amino acid sequence of a molecule (possibly an unknown molecule) against the amino acid sequence of Pim-1; identifying conserved and variable regions by sequence or structure; generating structure coordinates for structurally conserved residues of the unknown structure from those of Pim-1; generating conformations for the structurally variable residues in the unknown structure; replacing the non-conserved residues of Pim-1 with residues in the unknown structure; building side chain conformations; and refining and/or evaluating the unknown structure.

[0141] Software programs that are useful in homology modeling include XALIGN (Wishart et al., *Comput. Appl. Biosci.* 10: 687-88 (1994)) and CLUSTAL W Alignment

Tool, Higgins et al., *supra*. See also, U.S. Patent No. 5,884,230. These references are incorporated herein by reference.

[0142] To perform the sequence alignment, programs such as the "bestfit" program available from the Genetics Computer Group (Waterman in *Advances in Applied Mathematics* 2: 482 (1981), which is incorporated herein by reference) and CLUSTAL W Alignment Tool (Higgins et al., *supra*, which is incorporated by reference) can be used. To model the amino acid side chains of homologous molecules, the amino acid residues in Pim-1 can be replaced, using a computer graphics program such as "O" (Jones et al., (1991) *Acta Cryst. Sect. A* 47: 110-119), by those of the homologous protein, where they differ. The same orientation or a different orientation of the amino acid can be used. Insertions and deletions of amino acid residues may be necessary where gaps occur in the sequence alignment. However, certain portions of the active site of Pim-1 and its homologues are highly conserved with essentially no insertions and deletions.

[0143] Homology modeling can be performed using, for example, the computer programs SWISS-MODEL available through Glaxo Wellcome Experimental Research in Geneva, Switzerland; WHATIF available on EMBL servers; Schnare et al., *J. Mol. Biol.* 256: 701-719 (1996); Blundell et al., *Nature* 326: 347-352 (1987); Fetrow and Bryant, *Bio/Technology* 11:479-484 (1993); Greer, *Methods in Enzymology* 202: 239-252 (1991); and Johnson et al., *Crit. Rev. Biochem. Mol. Biol.* 29:1-68 (1994). An example of homology modeling can be found, for example, in Szklarz G.D., *Life Sci.* 61: 2507-2520 (1997). These references are incorporated herein by reference.

[0144] Thus, in accordance with the present invention, data capable of generating the three-dimensional structure or three-dimensional representation of the above molecules or molecular complexes, or binding pockets thereof, can be stored in a machine-readable storage medium, which is capable of displaying structural information or a graphical three-dimensional representation of the structure. In one embodiment, the means of generating three-dimensional information is provided by the means for generating a three-dimensional structural representation of the binding pocket or protein of a molecule or molecular complex.

Rational Drug Design

[0145] The Pim-1 structure coordinates or the three-dimensional graphical representation generated from these coordinates may be used in conjunction with a computer for a variety of purposes, including drug discovery.

[0146] For example, the structure encoded by the data may be computationally evaluated for its ability to associate with chemical entities. Chemical entities that associate with Pim-1 may inhibit or activate Pim-1 or its homologues, and are potential drug candidates. Alternatively, the structure encoded by the data may be displayed in a graphical three-dimensional representation on a computer screen. This allows visual inspection of the structure, as well as visual inspection of the structure's association with chemical entities.

[0147] In one embodiment, the invention provides for a method of using a computer for selecting an orientation of a chemical entity that interacts favorably with a binding pocket or protein comprising the steps of:

(a) providing the structure coordinates of said binding pocket or protein on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) employing computational means to dock a first chemical entity in the binding pocket or protein;

(c) quantifying the association between said chemical entity and all or part of the binding pocket or protein for different orientations of the chemical entity; and

(d) selecting the orientation of the chemical entity with the most favorable interaction based on said quantified association.

[0148] In one embodiment, the docking is facilitated by said quantified association.

[0149] In one embodiment, the above method further comprises the following steps before step (a):

(e) producing a crystal of a molecule or molecular complex comprising Pim-1 or homologue thereof;

(f) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal; and

(g) identifying all or part of a binding pocket that corresponds to said binding pocket.

[0150] Three-dimensional structural information in step (a) may be generated by instructions such as a computer program or commands that can generate a three-dimensional representation; subtract distances between atoms; calculate chemical energies for a Pim-1 molecule, molecular complex or homologues thereof; or calculate or minimize the chemical energies of an association of Pim-1 molecule, molecular complex or homologues thereof to a chemical entity. These types of computer programs are known in the art. The graphical representation can be generated or displayed by commercially available software programs. Examples of software programs include but are not limited to QUANTA (Accelrys, San Diego, CA ©2001, 2002), O (Jones *et al.*, *Acta Crystallogr.* A47: 110-119 (1991)) and RIBBONS (Carson, *J. Appl. Crystallogr.* 24: 958-961 (1991)), which are incorporated herein by reference. Certain software programs may imbue this representation with physico-chemical attributes which are known from the chemical composition of the molecule, such as residue charge, hydrophobicity, torsional and rotational degrees of freedom for the residue or segment, etc. Examples of software programs for calculating chemical energies are described below.

[0151] The above method may further comprise the following step after step (d): outputting said quantified association to a suitable output hardware, such as a CRT display terminal, a CD or DVD recorder, ZIP™ or JAZ™ drive, a disk drive, or other machine-readable data storage device, as described previously. The method may further comprise generating a three-dimensional structure, graphical representation thereof, or both, of the molecule or molecular complex prior to step (b).

[0152] One embodiment of this invention provides for the above method, wherein energy minimization, molecular dynamics simulations, or rigid body minimizations are performed simultaneously with or following step (b).

[0153] The above method may further comprise the steps of:

(e) repeating steps (b) through (d) with a second chemical entity; and

(f) selecting at least one of said first or second chemical entity that interacts more favorably with said binding pocket or protein based on said quantified association of said first or second chemical entity.

[0154] In another embodiment, the invention provides for the method of using a computer for selecting an orientation of a chemical entity with a favorable shape complementarity in a binding pocket comprising the steps of:

(a) providing the structure coordinates of said binding pocket and all or part of the ligand bound therein on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) employing computational means to dock a first chemical entity in the binding pocket;

(c) quantitating the contact score of said chemical entity in different orientations; and

(d) selecting an orientation with the highest contact score.

[0155] In one embodiment, the docking is facilitated by the contact score.

[0156] The method above may further comprise the step of generating a three-dimensional graphical representation of the binding pocket and all or part of the ligand bound therein prior to step (b).

[0157] The method above may further comprise the steps of:

(e) repeating steps (b) through (d) with a second chemical entity; and

(f) selecting at least one of said first or second chemical entity that has a higher contact score based on said quantitated contact score of said first or second chemical entity.

[0158] In another embodiment, the invention provides a method for screening a plurality of chemical entities to associate at a deformation energy of binding of less than –7 kcal/mol with said binding pocket:

(a) employing computational means, which utilize said structure coordinates to dock one of said plurality of chemical entities in said binding pocket;

(b) quantifying the deformation energy of binding between the chemical entity and the binding pocket;

(c) repeating steps (a) and (b) for each remaining chemical entity; and

(d) outputting a set of chemical entities that associate with the binding pocket at a deformation energy of binding of less than –7 kcal/mol to a suitable output hardware.

[0159] In another embodiment, the method comprises the steps of:

(a) constructing a computer model of a binding pocket of a molecule or molecular complex;

(b) selecting a chemical entity to be evaluated by a method selected from the group consisting of assembling said chemical entity; selecting a chemical entity from a small molecule database; de novo ligand design of said

chemical entity; and modifying a known agonist or inhibitor, or a portion thereof, of a Pim-1 protein, or homologue thereof;

(c) employing computational means to dock said chemical entity to be evaluated in said binding pocket in order to provide an energy-minimized configuration of said chemical entity in the binding pocket; and

(d) evaluating the results of said docking to quantify the association between said chemical entity and the binding pocket.

[0160] Alternatively, the structure coordinates of the Pim-1 binding pockets may be utilized in a method for identifying a candidate inhibitor of a molecule or molecular complex comprising a binding pocket of Pim-1. This method comprises the steps of:

(a) using a three-dimensional structure of the binding pocket or protein to design, select or optimize a plurality of chemical entities;

(b) contacting each chemical entity with the molecule and molecular complex;

(c) monitoring the inhibition to the catalytic activity of the molecule or molecular complex by the chemical entity; and

(d) selecting a chemical entity based on the effect of the chemical entity on the activity of the molecule or molecular complex.

[0161] In one embodiment, the three-dimensional structure is displayed as a graphical representation.

[0162] In another embodiment, the method comprises the steps of:

(a) constructing a computer model of a binding pocket of the molecule or molecular complex;

(b) selecting a chemical entity to be evaluated by a method selected from the group consisting of assembling said chemical entity; selecting a

chemical entity from a small molecule database; de novo ligand design of said chemical entity; and modifying a known agonist or inhibitor, or a portion thereof, of a Pim-1 protein or homologue thereof;

(c) employing computational means to dock said chemical entity to be evaluated and said binding pocket in order to provide an energy-minimized configuration of said chemical entity in the binding pocket; and

(d) evaluating the results of said docking to quantify the association between said chemical entity and the binding pocket;

(e) synthesizing said chemical entity; and

(f) contacting said chemical entity with said molecule or molecular complex to determine the ability of said chemical entity to activate or inhibit said molecule.

[0163] In one embodiment, the invention provides a method of designing a compound or complex that associates with all or part of the binding pocket comprising the steps of:

(a) providing the structure coordinates of said binding pocket or protein on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) using the computer to dock a first chemical entity in part of the binding pocket or protein;

(c) docking a second chemical entity in another part of the binding pocket or protein;

(d) quantifying the association between the first and second chemical entity and part of the binding pocket or protein;

(e) repeating steps (b) to (d) with another first and second chemical entity, selecting a first and a second chemical entity based on said quantified association of all of said first and second chemical entity;

(f) optionally, visually inspecting the relationship of the first and second chemical entity to each other in relation to the binding pocket or protein on a computer screen using the three-dimensional graphical representation of the binding pocket or protein and said first and second chemical entity; and

(g) assembling the first and second chemical entity into a compound or complex that interacts with said binding pocket by model building.

[0164] For the first time, the present invention permits the use of molecular design techniques to identify, select and design chemical entities, including inhibitory compounds, capable of binding to Pim-1 or Pim-1-like binding pockets, motifs and domains.

[0165] Applicants' elucidation of binding pockets on Pim-1 provides the necessary information for designing new chemical entities and compounds that may interact with Pim-1 substrate, active site, ligand binding pockets or Pim-1-like substrate, active site or ligand binding pockets, in whole or in part.

[0166] Throughout this section, discussions about the ability of a chemical entity to bind to, interact with or inhibit Pim-1 binding pockets refer to features of the entity alone.

[0167] The design of compounds that bind to or inhibit Pim-1 binding pockets according to this invention generally involves consideration of two factors. First, the chemical entity must be capable of physically and structurally associating with parts or all of the Pim-1 binding pockets. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions and electrostatic interactions.

[0168] Second, the chemical entity must be able to assume a conformation that allows it to associate with the Pim-1 binding pockets directly. Although certain

portions of the chemical entity will not directly participate in these associations, those portions of the chemical entity may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, or the spacing between functional groups of a chemical entity comprising several chemical entities that directly interact with the Pim-1 or Pim-1-like binding pockets.

[0169] The potential inhibitory or binding effect of a chemical entity on Pim-1 binding pockets may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given entity suggests insufficient interaction and association between it and the Pim-1 binding pockets, testing of the entity is obviated. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to a Pim-1 binding pocket. This may be achieved by testing the ability of the molecule to inhibit Pim-1 using the assays described in Example 5 and Fox et al., , *Protein Sci.* 7: 2249-2255 (1998), which is incorporated herein by reference.

[0170] A potential inhibitor of a Pim-1 binding pocket may be computationally evaluated by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the Pim-1 binding pockets.

[0171] One skilled in the art may use one of several methods to screen chemical entities or fragments or moieties thereof for their ability to associate with the binding pockets described herein. This process may begin by visual inspection of, for example, any of the binding pockets on the computer screen based on the Pim-1 structure coordinates Figures 1A, 2A or 3A, or other coordinates which define a similar shape generated from the machine-readable storage medium. Selected chemical entities, or fragments or moieties thereof may then be positioned in a variety of orientations, or docked, within that binding pocket as defined *supra*. Docking may be accomplished using software such as QUANTA (Accelrys, San Diego, CA ©2001, 2002) and Sybyl (Tripos Associates, St. Louis, MO), followed by, or performed simultaneously with, energy minimization, rigid-body minimization (Gshwend,

supra) and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

[0172] Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

1. GRID (Goodford, P. J., "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", *J. Med. Chem.* 28: 849-857 (1985)). GRID is available from Oxford University, Oxford, UK.

2. MCSS (Miranker et al., "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." *Proteins Struct. Funct. Genet.* 11: 29-34 (1991)). MCSS is available from Molecular Simulations, San Diego, CA.

3. AUTODOCK (Goodsell et al., "Automated Docking of Substrates to Proteins by Simulated Annealing", *Proteins Struct. Funct. and Genet.* 8: 195-202 (1990)). AUTODOCK is available from Scripps Research Institute, La Jolla, CA.

4. DOCK (Kuntz et al., "A Geometric Approach to Macromolecule-Ligand Interactions", *J. Mol. Biol.* 161: 269-288 (1982)). DOCK is available from University of California, San Francisco, CA.

[0173] Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of Pim-1. This would be followed by manual model building using software such as QUANTA (Accelrys, San Diego, CA ©2001, 2002) or Sybyl (Tripos Associates, St. Louis, MO).

[0174] Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT (Bartlett et al., "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in *Molecular Recognition in Chemical and Biological Problems*,.S.M. Roberts, Ed., Royal Society of Chemistry, Special Publication No. 78: pp. 182-196 (1989); Lauri, G. and Bartlett,P.A., "CAVEAT: A Program to Facilitate the Design of Organic Molecules", *J. Comp. Aid. Molec. Design* 8: 51-66 (1994)). CAVEAT is available from the University of California, Berkeley, CA.

2. 3D Database systems such as ISIS (MDL Information Systems, San Leandro, CA). This area is reviewed in Martin, Y. C., "3D Database Searching in Drug Design", *J. Med. Chem.* 35: 2145-2154 (1992).

3. HOOK (Eisen et al., "HOOK: A Program for Finding Novel Molecular Architectures that Satisfy the Chemical and Steric Requirements of a Macromolecule Binding Site", *Proteins Struct. Funct. Genet.* 19: 199-221 (1994)). HOOK is available from Molecular Simulations, San Diego, CA.

[0175] Instead of proceeding to build an inhibitor of a Pim-1 binding pocket in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other Pim-1 binding compounds may be designed as a whole or "de novo" using either an empty binding pocket or optionally including some portion(s) of a known inhibitor(s). There are many de novo ligand design methods including:

1. LUDI (Böhm, H.-J., "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", *J. Comp. Aid. Molec. Design* 6: pp. 61-78 (1992)). LUDI is available from Molecular Simulations Incorporated, San Diego, CA.

2. LEGEND (Nishibata et al., *Tetrahedron* 47: 8985-8990 (1991)). LEGEND is available from Molecular Simulations Incorporated, San Diego, CA.

3. LeapFrog (available from Tripos Associates, St. Louis, MO).

4. SPROUT (Gillet et al., "SPROUT: A Program for Structure Generation)", *J. Comp. Aid. Molec. Design* 7: 127-153 (1993)). SPROUT is available from the University of Leeds, UK.

[0176] Other molecular modeling techniques may also be employed in accordance with this invention (see, e.g., Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, *J. Med. Chem.* 33: 883-894 (1990); see also, Navia, M. A. and Murcko, M. A., "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology 2: 202-210 (1992); Balbes et al., "A Perspective of Modern Methods in Computer-Aided Drug Design", in *Reviews in Computational Chemistry*, K. B. Lipkowitz and D. B. Boyd, Eds., VCH Publishers, New York, 5: pp. 337-379 (1994); see also, Guida, W.C., "Software For Structure-Based Drug Design", *Curr. Opin. Struct. Biology* 4: 777-781 (1994)).

[0177] Once a chemical entity has been designed or selected by the above methods, the efficiency with which that entity may bind to any of the above binding pockets may be tested and optimized by computational evaluation. For example, an effective binding pocket inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient binding pocket inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, more preferably, not greater than 7 kcal/mole. Binding pocket inhibitors may interact with the binding pocket in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the inhibitor binds to the protein.

[0178] A chemical entity designed or selected as binding to any one of the above binding pocket may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme and with the surrounding water molecules. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions.

[0179] Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interactions. Examples of programs designed for such uses include: Gaussian 94, revision C (M. J. Frisch, Gaussian, Inc., Pittsburgh, PA ©1995); AMBER, version 4.1 (P. A. Kollman, University of California at San Francisco, ©1995); QUANTA/CHARMM (Accelrys, San Diego, CA ©2001, 2002); Insight II/Discover (Molecular Simulations, Inc., San Diego, CA ©1998); DelPhi (Molecular Simulations, Inc., San Diego, CA ©1998); and AMSOL (Quantum Chemistry Program Exchange, Indiana University). These programs may be implemented, for instance, using a Silicon Graphics workstation such as an Indigo2 with "IMPACT" graphics. Other hardware systems and software packages will be known to those skilled in the art.

[0180] Another approach enabled by this invention is the computational screening of small molecule databases for chemical entities or compounds that can bind in whole, or in part, to any of the above binding pocket. In this screening, the quality of fit of such entities to the binding pocket may be judged either by shape complementarity or by estimated interaction energy (Meng et al., *J. Comp. Chem.* 13: 505-524 (1992)).

[0181] Another particularly useful drug design technique enabled by this invention is iterative drug design. Iterative drug design is a method for optimizing associations between a protein and a chemical entity by determining and evaluating the three-dimensional structures of successive sets of protein/chemical entity complexes.

[0182] In iterative drug design, crystals of a series of protein or protein complexes are obtained and then the three-dimensional structures of each crystal is solved. Such an approach provides insight into the association between the proteins and compounds of each complex. This is accomplished by selecting compounds with inhibitory activity, obtaining crystals of this new protein/compound complex, solving the three-dimensional structure of the complex, and comparing the associations between the new protein/compound complex and previously solved protein/compound complexes. By observing how changes in the compound affected the protein/compound associations, these associations may be optimized.

[0183] In some cases, iterative drug design is carried out by forming successive protein-compound complexes and then crystallizing each new complex. High throughput crystallization assays may be used to find a new crystallization condition or to optimize the original protein crystallization condition for the new complex. Alternatively, a pre-formed protein crystal may be soaked in the presence of an inhibitor, thereby forming a protein/compound complex and obviating the need to crystallize each individual protein/compound complex.

[0184] Any of the above methods may be used to design peptide or small molecule which may have inhibitory effects on full-length Pim-1 protein or fragments thereof, or on full-length Pim-1 protein which is mutated in or fragments of the mutated protein thereof.

Structure Determination of Other Molecules

[0185] The structure coordinates set forth in Figures 1A, 2A or 3A can also be used in obtaining structural information about other crystallized molecules or molecular complexes. This may be achieved by any of a number of well-known techniques, including molecular replacement.

[0186] According to one embodiment, the machine-readable data storage medium comprises a data storage material encoded with a first set of machine readable data which comprises the Fourier transform of at least a portion of the structure coordinates set forth in Figures 1A, 2A or 3A or homology model thereof, and which, when using a machine programmed with instructions for using said data, can be combined with a second set of machine readable data comprising the X-ray diffraction pattern of a molecule or molecular complex to determine at least a portion of the structure coordinates corresponding to the second set of machine readable data.

[0187] In another embodiment, the invention provides a computer for determining at least a portion of the structure coordinates corresponding to X-ray diffraction data obtained from a molecule or molecular complex having an unknown structure, wherein said computer comprises:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structure coordinates of Pim-1 according to Figures 1A, 2A or 3A or homology model thereof;

(b) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises X-ray diffraction data obtained from said molecule or molecular complex having an unknown structure; and

(c) instructions for performing a Fourier transform of the machine-readable data of (a) and for processing said machine-readable data of (b) into structure coordinates.

[0188] For example, the Fourier transform of at least a portion of the structure coordinates set forth in Figures 1A, 2A or 3A or homology model thereof may be used to determine at least a portion of the structure coordinates of the molecule or molecular complex.

[0189] Therefore, in another embodiment this invention provides a method of utilizing molecular replacement to obtain structural information about a molecule or a molecular complex of unknown structure, wherein the molecule or molecular complex is sufficiently homologous to Pim-1, comprising the steps of:

(a) crystallizing said molecule or molecular complex of unknown structure;

(b) generating X-ray diffraction data from said crystallized molecule or molecular complex;

(c) applying at least a portion of the Pim-1 structure coordinates set forth in one of Figures 1A, 2A or 3A or a homology model thereof to the X-ray diffraction data to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown; and

(d) generating a structural model of the molecule or molecular complex from the three-dimensional electron density map.

[0190] In one embodiment, the method is performed using a computer. In another embodiment, the molecule is selected from the group consisting of Pim-1 protein and Pim-1 protein homologues. In another embodiment, the molecular complex is Pim-1 protein complex or homologue thereof.

[0191] By using molecular replacement, all or part of the structure coordinates of Pim-1 as provided by this invention (and set forth in Figures 1A, 2A or 3A) can be used to determine the structure of a crystallized molecule or molecular complex whose structure is unknown more quickly and efficiently than attempting to determine such information *ab initio*.

[0192] Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that can not be determined directly. Obtaining accurate values for the phases, by methods other than molecular replacement, is a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure may provide a satisfactory estimate of the phases for the unknown structure.

[0193] Thus, this method involves generating a preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of Pim-1 protein according to Figure 1A, 2A or 3A within the unit cell of the crystal of the unknown molecule or molecular complex so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model building and structure refinement techniques to provide a final, accurate structure of the unknown

crystallized molecule or molecular complex (E. Lattman, "Use of the Rotation and Translation Functions", in *Meth. Enzymol.* 115: 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser. No. 13, Gordon & Breach, New York (1972)).

[0194] The structure of any portion of any crystallized molecule or molecular complex that is sufficiently homologous to any portion of the structure of human Pim-1 protein can be resolved by this method.

[0195] In one embodiment, the method of molecular replacement is utilized to obtain structural information about a Pim-1 homologue. The structure coordinates of Pim-1 as provided by this invention are particularly useful in solving the structure of Pim-1 complexes that are bound by ligands, substrates and inhibitors.

[0196] Furthermore, the structure coordinates of Pim-1 as provided by this invention are useful in solving the structure of Pim-1 proteins that have amino acid substitutions, additions and/or deletions (referred to collectively as "Pim-1 mutants", as compared to naturally occurring Pim-1). These Pim-1 mutants may optionally be crystallized in co-complex with a chemical entity. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type Pim-1. Potential sites for modification within the various binding pockets of the enzyme may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between Pim-1 and a chemical entity or compound.

[0197] The structure coordinates are also particularly useful in solving the structure of crystals of Pim-1 or homologues co-complexed with a variety of chemical entities. This approach enables the determination of the optimal sites for interaction between chemical entities, including candidate Pim-1 inhibitors. For example, high resolution X-ray diffraction data collected from crystals exposed to different types of solvent allows the determination of where each type of solvent molecule resides. Small

molecules that bind tightly to those sites can then be designed and synthesized and tested for their Pim-1 inhibition activity.

[0198] All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined using 1.5-3.4 Å resolution X-ray data to an R value of about 0.30 or less using computer software, such as X-PLOR (Yale University, ©1992, distributed by Molecular Simulations, Inc.; see, e.g., Blundell & Johnson, *supra*; *Meth. Enzymol.* vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985)) or CNS (Brunger et al., *Acta Cryst.* D54: 905-921, (1998)).

[0199] In order that this invention be more fully understood, the following examples are set forth. These examples are for the purpose of illustration only and are not to be construed as limiting the scope of the invention in any way.

Example 1: Cloning and Expression of Pim-1

[0200] Full-length Pim-1 (residues M1-K313) was cloned in two parts by PCR from a human IMAGE Consortium clone (GenBank GI 1845036), and from a human bone marrow cDNA library (BD Biosciences, Clontech, Palo Alto, CA). The pieces were fused by PCR and inserted into the NdeI and EcoRI sites of the dual promoter vector pBEV1, encoding a protein with an N-terminal HexaHis tag and thrombin cleavage site. The amino acid sequence of this Pim-1 clone is identical to SwissProt entry P11309.

[0201] BL21/DE3 pLysS *E. coli* cells were transformed with the construct encoding full-length human Pim-1 kinase, using a standard transformation protocol (Stratagene, La Jolla, CA). Freshly transformed cells were grown at 37 °C in Brain Heart Infusion Medium (DIFCO laboratories, Detroit, MI) supplemented with 100 μg/ml carbenicillin and 35 μg/ml chloramphenicol. Cells were grown at 37 °C to an optical density of 0.75 at 600 nm, and expression was induced at 28 °C with 1 mM IPTG. Cells were harvested via centrifugation 4 hours post-induction and flash frozen at –80 °C prior to purification.

Example 2: Purification of Pim-1

[0202] Frozen cell pellets (~30 g) were thawed in 7 volumes of Buffer A (50 mM HEPES 7.8, 300 mM NaCl, 10% (v/v) glycerol, 3 mM β-mercaptoethanol) containing 0.1% (v/v) Tween-20, 50 μM DFP, 1 μg/ml E-64, 1 μg/ml leupeptin and 10 μg/ml pepstatin (Roche Diagnostics Corp, Indianapolis, IN) and lysed in a microfluidizer (Microfluidics, Newton, MA). The lysate was centrifuged at 54,000 x g for 45 min and the supernatant was incubated with 1 ml of TALON™ metal affinity resin (BD Biosciences, Clontech) per 5 mg of protein overnight at 4 °C. The resin was washed with 20 column volumes of Buffer A and the Pim-1 protein was eluted with Buffer A containing 100 mM imidazole. Fractions containing Pim-1 were pooled and concentrated by ultrafiltration using a 30 KDa molecular weight cut-off (MWCO) membrane in an Amicon stirred-cell concentrator (Millipore, Billerica, MA).

[0203] The concentrated fractions of Pim-1 was then loaded onto a Superdex 200 column (90 x 2.6 cm, Amersham Bioscience Corp, Uppsala, Sweden) that was equilibrated in Buffer B (50 mM HEPES pH 7.8, 200 mM NaCl, 10% (v/v) glycerol, and 5 mM β-mercaptoethanol). Fractions were pooled based on SDS-PAGE, diluted to 25 mM NaCl with 50 mM HEPES, pH 7.8, 10% (v/v) glycerol and 5 mM dithiothreitol (DTT), and loaded onto a Pharmacia 8 ml pre-packed MonoQ (HR 10/10) anion-exchange column (Amersham Bioscience Corp, Uppsala, Sweden) that was equilibrated in Buffer C (50 mM HEPES pH 7.8, 20 mM NaCl, 10% (v/v) glycerol, 5 mM DTT). Pim-1 was eluted using a gradient of 0-40% Buffer D (buffer C plus 1 M NaCl) over 60 column volumes. Peak fractions were collected as four separate pools (I-IV) based on the elution chromatogram. Pim-1 was dialyzed into 20 mM Tris pH 8.0 (25 °C), 100 mM NaCl, 5 mM DTT and concentrated to 10 mg/ml using a 10 KDa MWCO Vivaspin concentrator (Vivascience, Hanover, Germany). The identity of the purified Pim-1 was confirmed by N-terminal amino acid sequencing.

[0204] After sequential purification with affinity and size exclusion chromatography, the Pim-1 protein was >98% pure, but was heterogeneous with respect to phosphorylation states. Typically, preparations contained a mixture of species with 0-5 phosphoryl groups, which were partially resolved by anion exchange

chromatography. Purified Pim-1 had a monomer:dimer ratio of 80:20 (Kd 23 μM; apparent molecular weight of the monomer 44,023 Da) as determined by analytical ultracentrifugation and was completely free of higher molecular weight oligomers.

[0205] Pim-1 crystallized from different MonoQ pools gave similar crystal forms. Phosphoamino acid analysis revealed that Pim-1 purified from *E.coli* was extensively phosphorylated in the HexaHis tag (MGSSHHHHHHSSGLVPRGSH) (SEQ ID NO: 6) and the four MonoQ pools differed mainly in the degree of phosphorylation in this region. Dephosphorylation of Pim-1 with Lambda phosphatase (New England Biolabs) followed by autophosphorylation showed that Pim-1 readily autophosphorylates in the HexaHis tag region. Ser261 was the major phosphorylation site observed in Pools III and IV. Other minor phosphorylation sites, Ser8, Thr23 and Ser98 were present to varying degrees in each pool.

[0206] Kinase activity of MonoQ pools I-IV was tested using S6 peptide as a substrate. All four pools showed very similar kinetic parameters (k_{cat} = 4±0.4 s^{-1}; peptide K_m =51±2 μM and ATP K_m =120±16 μM), despite of the fact that they were phosphorylated to a different degree at several sites. A panel of kinase inhibitors was evaluated for their ability to inhibit Pim-1. Staurosporine and structurally similar compounds, such as K-252a and bisindolyl-maleimides-I and –IX, were found to inhibit Pim-1 with sub-micromolar potency (Table 1). These compounds are non-specific inhibitors of Ser/Thr and Tyr kinases (Dumas, J., *J. Exp. Opin. Ther. Patents* 11: 405-429 (2001); Cohen, P. *Nat. Rev. Drug Discov.* 1: 309-315 (2002); Hashimoto et al., *Biochem. Biophys. Res. Commun.* 181: 423-429 (1991); Harris et al., *Biochem. Biophys. Res. Commun.* 227: 672-676 (1996); Davies et al., *Biochem. J.* 351: 95-105 (2000); Berg et al., *J. Biol. Chem.* 267: 13-16 (1992); Mizuno et al., *FEBS Lett.* 330: 114-116 (1993)). LY294002 was found to be a potent inhibitor of Pim-1 with IC_{50}=4 μM. This compound was originally described as a specific inhibitor of PI3K with 1.4 μM IC_{50} (Mizuno et al., *FEBS Lett.* 330: 114-116 (1993)). Later, Davies et al (Davies et al., *supra*) reported that LY294002 inhibits PI3K and Casein kinase 2 with a similar potency (10 μM and 6.9 μM, respectively).

Example 3: Analytical Ultracentrifugation Sedimentation Velocity Data Acquisition and Analysis

[0207] All sedimentation velocity experiments were performed with the Beckman Coulter Optima XL-I using an An60 Ti rotor and charcoal-filled Epon double-sector cells. A 400 µl aliquot of Pim-1 was loaded into the sample channel and 430 µl of buffer into the reference channel. Experiments were performed at 42,000 rpm for 8 h at 20 °C. Radial absorbance scans were collected in continuous scan mode at 280 nm every 10 min at a spacing of 0.001 cm. Velocity data were analyzed using DCDT+ (version 1.14) (Philo, J. S., *Anal. Biochem.* 279: 151-163 (2000)) and SVEDBERG (version 6.39) (Philo, J. S., *Biophys. J.* 72: 435-444 (1997)).

Example 4: Mass Spectrometric Analysis of Purified Pim-1

[0208] The overall phosphorylation state of each of the MonoQ purified pools I-IV of Pim-1 was determined by electrospray mass spectrometry of thrombin cleaved Pim-1. Electrospray mass spectra of protein samples were collected using a Micromass Quattro II triple quadrupole mass spectrometer (Waters Corp., Milford, MA) (Fox et al., , *FEBS Lett.* 461: 323-328 (1999)).

[0209] The phosphorylation sites of Pim-1 were identified from tryptic digests of the MonoQ purified pools I-IV to LC/MSMS on a QSTAR Pulsar quadrupole time-of-flight tandem mass spectrometer (AB/MDS-Sciex, Toronto, Canada) equipped with a nanoelectrospray ion source (MDS Protana, Odese, Denmark). Data were analyzed using the Mascot search engine (Matrix Science, London, UK).

Example 5: Kinase Assays

[0210] A coupled-enzyme assay (Fox et al., , *Protein Sci.* 7: 2249-2255 (1998)) was used to quantify the ADP generated in the kinase reaction with S6 peptide (RRRLSSLRA) (SEQ ID NO: 7) as a substrate. The assay was carried out in a total volume of 100 µl in 0.1 M HEPES buffer (pH 7.6) containing 10 mM $MgCl_2$, 2.5 mM phosphoenolpyruvate, 0.2 mM NADH, 30 µg/ml pyruvate kinase, 10 µg/ml lactate dehydrogenase (Roche Diagnostics Corp., Indianapolis, IN) and 2 mM DTT in a 96-well plate, and read at 340 nm at 30°C on a Spectramax spectrophotometer (Molecular

Devices, Sunnyvale, CA). Pim-1 concentration was 25 nM in all assays. The reaction was started by addition of ATP after 10 minutes pre-incubation of the reaction mixture at 30°C. Substrate concentrations were 1 mM S6 peptide, 2 mM ATP for activity assays and 40 μM S6 peptide, 100 μM ATP for IC_{50} determinations. Inhibitors were dissolved in DMSO and added to the reaction to 2.5% DMSO final at the beginning of pre-incubation period. Kinetic analysis was performed by non-linear regression fitting using the program Prism (GraphPad software, San Diego, CA, USA).

Example 6: Crystallization of Pim-1–adenosine complex

[0211] Pim-1 crystals were grown by the vapor diffusion method at 22 °C. Equal volumes of protein (12 mg/ml protein, 20 mM HEPES pH 8, 100 mM NaCl, 5 mM DTT) and well solution (1 M $(NH_4)_2HPO_4$, 100 mM citrate buffer pH 5.5, 200 mM NaCl) were mixed and suspended over 1 ml of well solution. Over 4 days, the crystals reached a final size of approximately 250 x 40 x 40 μm. Crystals were harvested and flash-frozen in a solution composed of the well solution with 30% (v/v) glycerol. A complex of Pim-1 with either staurosporine (Sigma-Aldrich, St. Louis, Missouri) or the inhibitor LY294002 (Calbiochem, La Jolla, California) was made by soaking apo crystals (grown as above) with 500 μM compound and 5% DMSO (final concentration) for 24 hours at room temperature. The adenosine - Pim-1 complex was made by adding adenosine (2 mM) to the protein prior to crystallization.

Example 7: X-ray Data Collection and Structure Determination

[0212] For the staurosporine and LY294002 complexes, X-ray diffraction data were recorded using a RU-200 X-ray generator and RaxisV++ detector (Rigaku, The Woodlands, Texas), and intensities were integrated and scaled using the program d*TREK (CrystalClear: An Integrated Program for the Collection and Processing of Area Detector Data, R. C., © 1997-2002; Pflugrath, *Acta Crystallogr.* D55: 1718-1725 (1999)). Diffraction data for the adenosine complex crystals were recorded at Beamline 5.0.2 at the Advanced Light Source (Lawrence Berkeley Laboratories, Berkeley, California). Intensities were integrated and scaled using the programs DENZO and SCALEPACK (Otwinowski, *supra*) and d*TREK (CrystalClear: An Integrated Program for the Collection and Processing of Area Detector Data, R. C., ©

1997-2002; Pflugrath, *Acta Crystallogr.* D55: 1718-1725 (1999)). Table 2 summarizes data collection.

[0213] The structure was determined by molecular replacement using homology models based upon phosphorylase kinase (PDB accession code 1PHK) (Owen et al., *supra*) and death-associated protein kinase (PDB accession code 1JKK) (Tereshko et al., *supra*). The molecular replacement solution was determined using AMoRe (Navaza, CCP4 distribution) (CCP4 (Collaborative Computational Project, N., *Acta Crystallogr.* D50: 760–763 (1994)). The crystals belong to the space group $P6_5$, and a single protein monomer comprises the asymmetric unit. The protein model was built using QUANTA (Accelrys, San Diego, CA ©2001, 2002) and refined with both CNX (Accelrys, San Diego, California) (Pannu, N. S., and Read, R. J., *Acta Crystallogr.* A 52: 659–668 (1996); Rice, L. M., and Brunger, A. T., *Proteins* 19: 277-290 (1994)) and BUSTER (Global Phasing Inc., Cambridge, UK) (Roversi et al., *Acta Crystallogr. D Biol. Crystallogr.* 56 (Pt 10): 1316-1323 (2000)).

[0214] Table 2 summarizes the Refinement Statistics. The refined models consist of the protein kinase catalytic domain. While full-length protein was used for crystallization (313 residues), 32 residues at the N-terminus, 8 residues at the C-terminus, and 4 residues in one loop (80-83) could not be built into the electron density. Glu79 was built as Ala because electron density was weak for the side chain of this amino acid residue. Phosphorylation of Ser261 is clearly visible in the electron density map. The phosphoserine side chain participates in both intra- and intermolecular interactions, and may be important in formation of the crystal packing interactions. Also, the electron density map reveals additional density adjacent to the sulfur of Cys161 indicating an adduct at this residue. The electron density was large enough to accommodate four non-hydrogen atoms; it was modeled as a β-mercaptoethanol adduct, however it is also consistent with a partially ordered DTT adduct. Both DTT and β-mercaptoethanol were used in the purification.

Example 8: Overview of Crystal Structure of Pim-1-Inhibitor Complexes

[0215] The structure of Pim-1 reveals a global fold typical of protein serine/threonine kinases, consisting of two domains linked by a hinge region (Figure 4). The smaller, N-terminal domain (residues 33-121) consists primarily of β-strands with one α-helix, and the C-terminal domain (residues 128-305) is largely α-helical. The active site is formed by a groove at the interface between these two domains, and is enclosed by the hinge region (residues 122-127), the glycine rich loop (residues 44-52), and the activation loop (residues 186-210). The Pim-1 structure was compared to several other protein kinases with high sequence homology such as c-AMP dependent kinase (PKA) and phosphorylase kinase (PHK). Pim-1 shares the same secondary and tertiary structure as other protein kinases. When secondary structural elements are aligned, a root mean square difference (RMSD) of 1.3 Å for C-α atom positions is observed between Pim-1 and both PKA or PHK (using 213 residues from PDB accession code 1PHK (Owen et al., *supra*) and 220 residues from PDB accession code 1ATP (Zheng et al., *Biochemistry* 32: 2154-2161 (1993)), respectively).

[0216] Among kinase structures, the conformation of the activation loop varies widely (reviewed in Huse, M., and Kuriyan, J., *Cell* 109: 275-282 (2002)). Many kinases are activated by phosphorylation in this region, causing a conformational change consistent with substrate binding. The Pim-1 activation loop is in a similar conformation to the active, peptide-bound form of PKA and the constitutively active kinase PHK. In PKA, Thr197 is phosphorylated and the conformation of the activated state is stabilized by a salt bridge to Arg165. In both Pim-1 and PHK, a similar salt bridge is observed, however, an acidic side chain takes the place of the phosphothreonine (Asp200-Arg166 in Pim-1, Glu182-Arg148 in PHK).

[0217] The positions and side chain rotamers of the catalytic residues resemble that observed in the PKA-ATP-peptide complex. In PKA, Asn171 forms a hydrogen bond to Asp166 and thus orients Asp166, which in turn forms a hydrogen bond with the substrate Ser or Thr hydroxyl group. The corresponding residues in Pim-1, Asn172 and Asp167, have the same position and side chain rotamers. Likewise, the residues of PKA which interact with the ATP phosphate or Mg^{2+} atoms (Lys72, Asn171, Asp184) are conserved both in sequence and position in Pim-1 (Lys67, Asn172,

Asp186). The conformation of the glycine rich loop (residues 45-52) in this structure differs from that of the PKA structures. The Pim-1 glycine rich loop moves toward the C-terminal domain and Phe49 adopts a rotamer in which the side chain points toward the hinge region, thereby filling the space usually occupied by ATP phosphates (Figure 6). A similar conformation has been observed in GSK-3β where Phe67 contacts the phosphate binding portion of the glycine rich loop (Bax et al., *Structure, (Camb)* 9: 1143-1152 (2001)).

[0218] The N- and C-terminal domains are connected by a hinge region, which forms important interactions with the adenine ring of ATP. Typically, the adenosine N1 nitrogen accepts a hydrogen bond from a main chain amide while the N6-amino atom donates a hydrogen bond to a main chain carbonyl. In the hinge region of Pim-1, however, the residue closest to the adenine N1 is a proline (Pro123), so a main chain amide is not available for this hydrogen bonding. A proline at this position is extremely rare: in fact, none of the kinases for which the structure is known has a similarly placed proline. Sequence alignments in the hinge region can be difficult because of low homology. The only other human kinases with a proline at this position are Pim-2, Pim-3, SgK069 and PRP4 (Manning et al., *Science* 298: 1912-1934 (2002)). This implies that the hydrogen bond to N1 of ATP is not necessary for substrate binding or catalysis in these kinases, and that other interactions are sufficient to correctly position ATP. Likewise, a kinase inhibitor optimized for Pim-1 selectivity would lack a hydrogen bond acceptor at the position corresponding to N1 of ATP, and might instead interact with the hinge via a van der Waal's contact.

[0219] The Pim-1 hinge sequence is also unusual due to a two-residue insertion relative to kinases such as CDK-2 (De Bondt et al., *Nature* 363: 595-602 (1993)) and JNK-3 (Xie et al., *Structure* 6: 983-991 (1998)), and a single residue insertion relative to PKA and Aurora (Cheetham et al., *J. Biol. Chem.* 277: 42419-42422 (2002)). A comparison of the hinge regions of Pim-1 and PKA is shown in Figure 5. Residues before and after the insertion superimpose well (Pim-1 residues 117-122 with PKA 117-122; Pim-1 128-131 with PKA 127-130). At the point of insertion (Pro125), the hinge bulges away from the ATP binding site by up to 4 Å. Some of the additional space created by the change in main chain position is occupied by the Val126 side

chain which is oriented toward the ATP binding pocket and interacts with Pro123. This unique hinge conformation could be utilized for the design of specific Pim-1 inhibitors, and creates a space for substitution at the position corresponding to C2 of ATP. For instance, polar interactions with the carbonyl oxygen of Pro123 or hydrophobic contacts with the side chain of Val126 would be unique to PIM.

[0220] One kinase which shares this two residue insertion is phosphoinositide 3-kinase (PI3K) (Walker et al., *Nature* 402: 313-320 (1999)). Overall, the structures of protein kinases and PI3K share many structural features, especially with respect to the ATP binding pocket. While there is little sequence homology in the hinge region between PI3K and Pim-1, the main chain conformations are remarkably similar (0.86 Å RMSD over 13 C-α positions). The PI3K and Pim-1 hinge conformation differ most at Pro125 (Asp884 in PI3K) (Figure 5).

Staurosporine Complex

[0221] The position of staurosporine bound to Pim-1 is similar to that found in other kinases. The compound is sandwiched between hydrophobic residues from the glycine rich loop (Ala65, Leu44, Val52, Phe49), the C-terminal domain (Ile104, Leu174, Ile185), and the hinge (Val126). A hydrogen bond is observed between the pyrrolidinone nitrogen and the Glu121 main chain carbonyl atom. The amino group of the staurosporine sugar moiety makes two hydrogen bonds: one to the main chain carbonyl of Glu171 and the other to the side chain oxygen of Asp128. Unlike other kinase-staurosporine complexes, no hydrogen bond is observed to the pyrrolidinone oxygen due to the presence of a proline at position 123. Compared to the PKA-staurosporine complex (PDB accession code 1STC) (Prade et al., *Structure* 5: 1627-1637 (1997)) , the staurosporine is rotated about 10° (about an axis perpendicular to the plane of the pyrrolidinone ring) toward the hinge, and into the additional space formed by the proline insertion in the hinge (Figure 5B). The aromatic rings of staurosporine in the Pim-1 and PKA structures are approximately coplanar. The relative position of the staurosporine in the two structures is, in part, fixed by the length of the side chain to which the sugar moiety forms a hydrogen bond (Asp128 in Pim-1, Glu128 in PKA).

[0222] A comparison of the staurosporine position in the Pim-1 and the PI3K complexes (PDB accession code 1E8Z) (Walker et al., *supra*; Pacold et al., *Cell* 103: 931-943 (2000)), reveals a shift and a rotation. In PI3K, two hydrogen bonds are made between the pyrrolidinone and the PI3K main chain, typical of other staurosporine complexes. Staurosporine bound to PI3K is shifted toward the outermost edge of the hinge by about 2.5 Å relative to the Pim-1 structure (Figure 5C). Also, the staurosporine is tilted about 30° about an axis parallel to the main chain of the hinge (between I879 and V882), such that the pyrrolidinone ring lies below (towards the C-terminal domain) the same ring in the Pim-1 structure (Figure 5D). While the conformations of the Pim-1 and PI3K hinges are similar, specific interactions with active site side chains bring about the difference in positions. For instance, in Pim-1, the side chain of Ala65 lies above the plane of the staurosporine pyrrolidinone ring. In PI3K, Ile831 occupies the same location in the active site, and the larger side chain causes the ring to tilt downwards, away from the glycine rich loop. Likewise, in Pim-1, the C-α carbon of Pro123 and the side chains of Ile104 and Val126 prevent staurosporine from adopting the same position seen in PI3K.

Adenosine Complex

[0223] In the Pim-1-adenosine complex, only a single hydrogen bond is observed with the hinge main chain: between the N6-amino group and the main chain carbonyl of Glu121. Relative to the PKA-adenosine complex (PDB accession code 1FMO) (Narayana et al., *Biochemistry* 36: 4438-4448 (1997)), the adenosine in Pim-1 rotates by approximately 20° toward the hinge (rotation axis perpendicular to the plane of the adenine ring, see Figure 5E). As with the staurosporine complex, the extent of the rotation is determined by the hydrogen bond acceptor at position 128.

[0224] In the PI3K-ATP complex structure (PDB accession code 1E8X), the adenine ring makes two hydrogen bonds to the main chain as seen in other protein kinases. However, the ATP bound to PI3K moves toward the hinge (Figure 5F) and tilts such that the adenine ring lies below the plane of the adenine ring in the Pim-1-adenosine complex (closer to the C-terminal domain). As described above, in Pim-1, the C-α of Pro123 prevents the adenine from moving to the position seen in PI3K.

LY294002 Complex

[0225] The structure of PI3K inhibitor LY294002 bound to Pim-1 (Figure 6A) was pursued based upon the observation of the compound's inhibitory activity in the Pim-1 *in vitro* assay as well as the conformational similarity between the Pim-1 and PI3K hinges. When bound to PI3K, the morpholine oxygen of LY294002 accepts a hydrogen bond from the amide nitrogen of Val882, making the same interaction as seen with N1 of ATP (PDB accession code 1E7V) (Figure 6B). The structure of the Pim-1-LY294002 complex reveals that compound orientation is quite different. Relative to the PI3K structure, the LY294002 compound rotates about 180° about the bond common to the 2 rings in the chromone. In this case, the only interaction with the hinge is a pair of hydrogen bonds between the main chain carbonyl of Glu121 and two aromatic hydrogens of the chromone (2.6 and 2.9 Å O to H distance). The chromone carbonyl oxygen makes a hydrogen bond to a solvent molecule, which in turn interacts with the main chain amide of Asp186. The phenyl group of LY294002 packs against the side chains of Arg122, Val 126 and Leu174, while the morpholine group interacts with Phe49 in the glycine-rich loop.

Phosphorylation of Pim-1

[0226] Pim-1 purified from *E.coli* was phosphorylated at Ser261 as well as multiple sites in the His-tag region. Palaty et al. (Palaty et al., *J. Biol. Chem.* 272: 10514-10521 (1997)) have identified Ser190 in Xenopus Pim-3 as the major autophosphorylation site and showed that Ser190Ala and Ser190Glu mutants are 7-fold less active than the wild type Pim-3. The equivalent residue in human Pim-1, Ser189, was not phosphorylated in the *E.coli* purified preparations. The fact that all four MonoQ Pim-1 pools exhibit very similar kinetic parameters indicates that the enzyme is constitutively active and that the phosphorylation state does not affect enzymatic activity. The specific activity (5 ± 0.2 μmol/min/mg) observed here is much higher than previously reported (Hoover et al., *supra*; Friedmann et al., *supra*; Palaty et al., *Biochem. Cell. Biol.* 75: 153-162 (1997); Palaty et al., *J. Biol. Chem.* 272: 10514-10521 (1997)). It is 60-fold greater than that reported by Friedman et al. for human GST-Pim-1 using a histone H1 peptide (KRRASGP) (Friedmann et al., *supra*; SEQ ID NO:8) and over 10^4-fold greater than that reported by Palaty et al. for

GST fusions of human Pim-1 using S6 peptide (AKRRRLSSLRA) (Palaty et al., *Biochem. Cell. Biol.* 75: 153-162 (1997); SEQ ID NO:9) . Since both studies utilized GST fusions for expression and purification, it is possible that this large protein tag had a detrimental effect on enzyme activity, either by interfering with substrate access to the active site, or with overall protein folding. Human Pim-1 described herein with a small HexaHis tag exhibited a substantially higher and physiologically relevant level of kinase activity.

Comparisons of Structures of Pim-1-inhibitor Complexes to Structures of Other Kinases

[0227] The overall structure and position of the catalytic residues of the Pim-1-adenosine complex represents the active state of the enzyme. The conformation of the activation loop resembles that of active kinases (PHK and phosphorylated PKA), consistent with the fact that Pim-1 is constitutively active. However, the structure of a Pim-1-ATP complex is likely to differ from the Pim-1-adenosine structures in the conformation of the glycine-rich loop and in the position of the adenosine. In the three ligand structures presented here, the side chain of Phe49 blocks the region of the active site normally occupied by the ATP phosphates. It is likely that ATP would displace Phe49, and the loop would adopt a more typical conformation. In GSK-3β, for instance, the corresponding phenylalanine residue is observed both within the active site pointing toward the hinge (Bax et al., *supra*) and, in another structure, outside the active site, pointing away from the hinge (ter Haar et al., *Nat. Struct. Biol.* 8: 593-596 (2001)).

[0228] The sequence and the conformation of the hinge region of Pim-1 differ from that found in other protein kinases: a conserved main chain hydrogen bond donor is replaced by a proline, and an insertion causes the hinge to bulge away from the adenine binding pocket. Nonetheless, Pim-1 is an active enzyme and binds compounds which also bind to other protein kinases (staurosporine, adenosine). Since the catalytic residues of Pim-1 are in the same position as in other protein kinases, and correct positioning of the phosphates of ATP is needed for catalysis, one would expect the position of the adenine and ribose to resemble that found in other kinases. Indeed, while the hinge conformation differs, the adenosine is bound in a similar way

as in PKA. It is likely that when Pim-1 binds ATP, as opposed to adenosine, interactions between the phosphates and catalytic residues would fix the position of ATP in a manner similar to PKA and other protein kinases.

[0229] While the hinge conformations between Pim-1 and PI3K are very similar, the positions of adenosine and staurosporine differ. In fact, the orientation of the ligands in Pim-1 more closely resembles that found in other protein kinases. The PI3K binding mode, characterized by the shift towards the hinge and tilt down toward the C-terminal domain, is sterically hindered in Pim-1. The presence of the C-α atom of Pro123 and the larger side chain at position 126 (valine instead of alanine), prevent the shift toward the hinge. The tilt toward the C-terminal domain is hindered by the side chain of Ile104 in Pim-1. In the absence of the conserved pair of hydrogen bonds to the hinge, a number of van der Waal's contacts constrain the position of the ligands.

[0230] The fact that LY294002 binds to Pim-1, a protein with a PI3K-like hinge, appears to be coincidental, since the compound orientation is quite different. While the proteins have structural similarities, none of the features in common contribute to the binding of LY294002. In fact, superposition of the two complexes reveals that the PI3K binding mode is sterically hindered by Pro123 in Pim-1. Also, the Pim-1 binding mode is incompatible with the PI3K structure: Trp182 in PI3K packs against the phenyl and the morpholine rings of LY294002, but would collide with the phenyl ring if the compound bound in the Pim-1 orientation.

[0231] The contacts between the Pim-1 hinge and LY294002 are quite unusual. Typically, ligands interact with the hinge via hydrogen bonds, where the donor hydrogen is bonded to either oxygen or nitrogen. In this case, only hydrogens bonded to aromatic carbon atoms interact with the hinge. If indeed these interactions were important for LY294002 binding, we would expect the arrangement of the atoms to be favorable for hydrogen bonding. The ideal (C)H to O distance is approximately 2.6-2.7 Å, and the distance between the Glu121 carbonyl and the LY294002 hydrogens is 2.6 and 2.9 Å. The ideal O--CH angle is 180°, but not less than 90°. The angles observed with LY294002 in Pim-1 are 140 and 130°. Further, the hydrogen and the peptide should be coplanar, which is the case in the Pim-1-LY294002 complex. It is

likely, therefore, that a pair of aromatic CH hydrogen bonds are formed between LY294002 and the Pim-1 hinge (Pierce et al., *Proteins*, 49: 567-576 (2002)).

[0232] The compound LY294002 is commonly used to assess the role of PI3K in cell signaling, and does not significantly inhibit most kinases (Davies et al., *supra*). For instance, PKA activity is reduced by only 9% (± 5%) in the presence of 50 μM LY294002, so we would not expect the structure of PKA to easily accommodate LY294002 binding. Indeed, both the Pim-1 and PI3K binding modes are sterically hindered by Thr183 and Val123, respectively, in PKA. One kinase inhibited by LY294002 is casein kinase 2 (CK2) (IC50 6.9 μM). The structures of CK2 and Pim-1 were aligned to predict how LY294002 might bind to CK2. The PI3K binding mode is blocked by the side chain of Val116 in CK2. However, the CK2 active site will accommodate LY294002 in the Pim-1 binding mode, with a 0.5 Å translation to avoid a close contact with Ile66.

[0233] In addition to kinases, LY294002 has also been observed to bind to proteins with unrelated sequences and functions. For instance, through a PI3K-independent mechanism, the compound has been shown to alter intracellular calcium concentrations in bronchial smooth muscle cells (Ethier, M. F., and Madison, J. M., *Cell, Calcium* 32: 31-38 (2002)), block the Kv2.1 and Kv1.4 channels (El-Kholy et al., *Faseb J.* 17: 720-722 (2003)), and also bind to and inhibit estrogen receptor (Pasapera Limon et al., *Mol. Cell. Endocrinol.* 200: 199-202 (2003)). This may be due to the fact that LY294002 is a relatively small, planar, and unelaborated molecule with several hydrogen bonding opportunities. It is likely that there are other, as yet, unidentified targets of this compound, and therefore LY294002 should be used with caution in cellular assays.

[0234] In protein kinases, the hinge conformation and the hydrogen bonds to ATP are highly conserved. The Pim-1 structure reveals how fairly standard substrate binding is achieved even when the hinge is unusual in both sequence and conformation. The structures of the adenosine and staurosporine complexes show how van der Waal's contacts play the same role as a conserved hydrogen bond in positioning the substrate. While the Pim-1 hinge closely resembles the analogous region in the active site of PI3K, the compound LY294002 interacts with the hinges

of the two proteins in very different ways. The Pim-1/LY294002 structure explains how LY294002 might inhibit other protein kinases, and this structure can be used to aid in the design of specific inhibitors, which utilize unique features of the Pim-1 active site.

[0235] While we have described a number of embodiments of this invention, it is apparent that our basic constructions may be altered to provide other embodiments which utilize the products, processes and methods of this invention.

Table 1. IC_{50} determination of some common kinase inhibitors

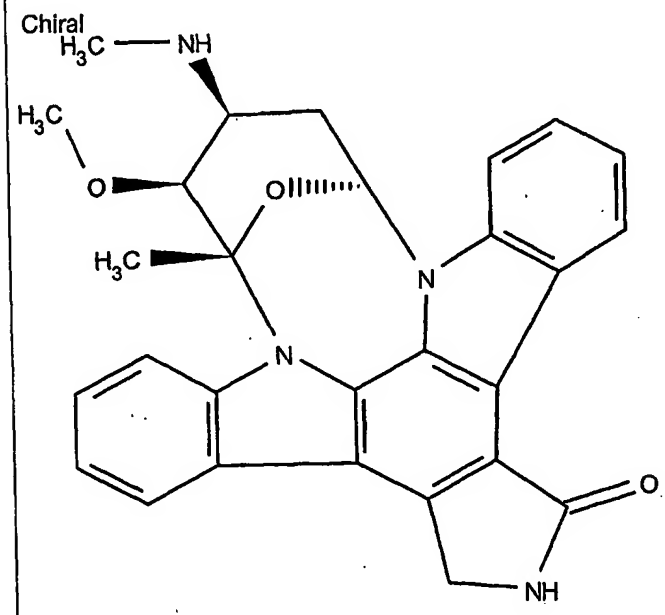
Inhibitor	IC_{50} (μM)	Reported Inhibition Targets
Staurosporine 	0.01	Broad-spectrum Ser/Thr and Tyr kinases (Cohen, *supra*; Hashimoto et al., *supra*)

Table 1. cont.

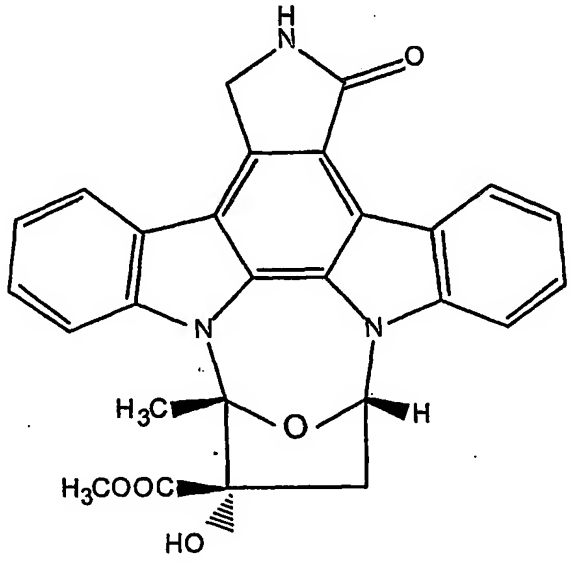
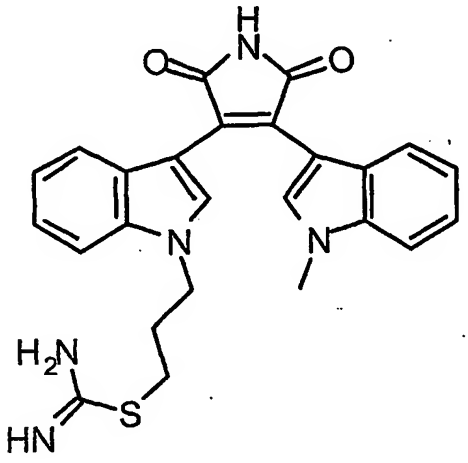
K-252a 	.15	Broad-spectrum Ser/Thr and Tyr kinases (Hashimoto et al., *supra;* Berg et al., *supra*; Mizuno et al., *supra*)
Bisindolyl-maleimide IX 	0.01	PKC, GSK3, MAPKAP-K1b, SGK, p70S6K (Harris et al., *supra;* Davies et al., *supra*)

Table 1. cont.

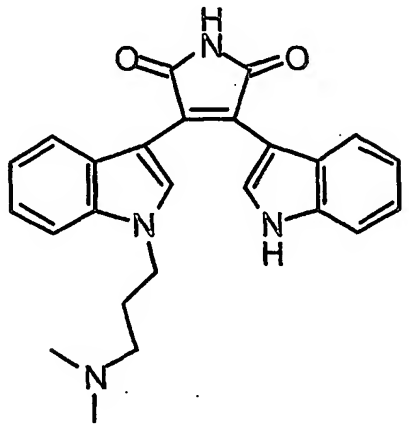
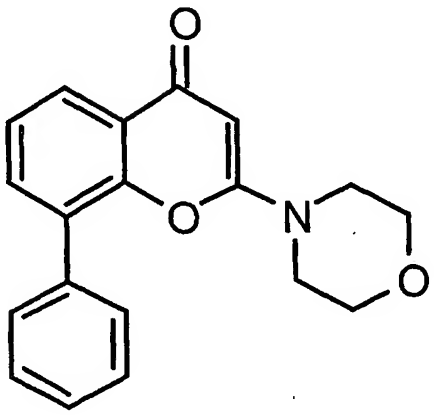
Bisindolyl-maleimide I 	0.15	PKC, MAPKAP-K1b, MSK1, p70S6K, GSK3 (Davies et al., *supra*)
LY294002 	4	PI3K, CK2 (Davies et al., *supra*; Vlahos et al., Davies et al., *supra*)

Table2: Data Collection and Refinement Statistics

Data set	Staurosporine	Adenosine	LY294002
Data collection			
X-ray source	Rigaku RU-H3R	ALS 5.0.2	Rigaku RU-H3R
Space group	$P6_5$	$P6_5$	$P6_5$
Unit cell parameters (Å)	a = b = 97.73		
c = 80.51	a = b = 98.27		
c = 80.39	a = b= 97.65		
c = 80.73			
Resolution (Å)	20 – 2.15	20 – 2.4	20 – 2.5
Unique reflections	22615	16430	14445
Redundancy	3.6	5.2	3.1
Completeness (%)*	94.9 (74.8)	94.3 (96.1)	94.9 (87.6)
R_{merge}*	0.050 (0.250)	0.060 (0.361)	0.072 (0.336)
$\langle I/\sigma \rangle$*	10.6 (2.3)	14.7 (3.9)	12.0 (2.6)
Refinement			
Reflections used	22526	16152	14206
Test reflections	1706	1268	1097
R-factor	0.205	0.210	0.208
Free R-factor (% data)	0.233 (7.6)	0.246 (7.9)	0.259 (7.7)
RMS deviation			
Bond lengths (Å)	0.015	0.007	0.009
Bond angles (°)	1.7	1.3	1.2
Dihedral angles (°)	23.1	22.8	22.2
Protein atoms	2202	2202	2202
Solvent atoms	142	81	136

*Values for the highest resolution shell are shown in parentheses.

$R_{merge} = \sum_{hkl} \sum_i |I(hkl)_i - \langle I(hkl) \rangle| / \sum_{hkl} \sum_i \langle I(hkl)_i \rangle$ over i observations of reflection hkl.

R-factor = $\sum ||F_{obs}| - |F_{calc}|| / \sum |F_{obs}|$ where F_{obs} and F_{calc} are the observed and calculated structure factors, respectively. Free R-factor is calculated from a randomly chosen subset of reflections not used for refinement.

CLAIMS

We Claim:

1. A crystal comprising a human Pim-1 protein.

2. A crystal comprising a Pim-1 homologue.

3. A crystal comprising a human Pim-1 protein complex.

4. A crystal comprising a Pim-1 homologue complex.

5. The crystal according to any one of claims 1 to 4, wherein said human Pim-1 protein, said Pim-1 homologue, said human Pim-1 protein complex, or said Pim-1 homologue complex is phosphorylated.

6. The crystal according to claim 3, wherein said human Pim-1 protein complex comprises human Pim-1 protein and a chemical entity selected from the group consisting of staurosporine, adenosine, 2-(4-morpholinyl)-8-phenyl-4H-1-benzopyran-4-one, ATP, an ATP analogue, a nucleotide triphosphate, a nucleotide diphosphate, phosphate and active site inhibitor.

7. The crystal according to claim 3, wherein said human Pim-1 protein complex comprises human Pim-1 protein and a chemical entity selected from the group consisting of staurosporine, adenosine, and 2-(4-morpholinyl)-8-phenyl-4H-1-benzopyran-4-one.

8. The crystal according to claim 2 or 4, wherein said Pim-1 homologue is amino acid residues 33-305 of SEQ ID NO:2.

9. A crystallizable composition comprising a human Pim-1 protein.

10. A crystallizable composition comprising a Pim-1 homologue.

11. A crystallizable composition comprising a human Pim-1 protein complex.

12. A crystallizable composition comprising a Pim-1 homologue complex.

13. The crystallizable composition according to any one claims 9 to 12, wherein said human Pim-1 protein, said Pim-1 homologue, said human Pim-1 protein complex, or said Pim-1 homologue complex is phosphorylated.

14. The crystallizable composition according to claim 11, wherein said human Pim-1 protein complex comprises human Pim-1 protein and a chemical entity selected from the group consisting of staurosporine, adenosine, 2-(4-morpholinyl)-8-phenyl-4H-1-benzopyran-4-one, ATP, an ATP analogue, a nucleotide triphosphate, a nucleotide diphosphate, phosphate and active site inhibitor.

15. The crystallizable composition according to claim 11, wherein said human Pim-1 protein complex comprises human Pim-1 protein and a chemical entity selected from the group consisting of staurosporine, adenosine, and 2-(4-morpholinyl)-8-phenyl-4H-1-benzopyran-4-one.

16. The crystallizable composition according to claim 10 or 12, wherein said Pim-1 homologue is amino acid residues 33-305 of SEQ ID NO:2.

17. A computer comprising:

(a) a machine-readable data storage medium, comprising a data storage material encoded with machine-readable data, wherein said data defines a binding pocket or protein selected from the group consisting of:

(i) a set of amino acid residues which are identical to human Pim-1 kinase amino acid residues Phe49, Ala65, Val126, and Leu174 according to Figure 1A, 2A or 3A, wherein the root mean square deviation of the backbone atoms between said amino acid residues and said human Pim-1 kinase amino acid residues which are identical is not greater than about 2.0 Å;

(ii) a set of amino acid residues comprising at least 8 amino acid residues which are identical to human Pim-1 kinase amino acid residues Leu44, Gly45, Phe49, Val52, Ala65, Lys67, Ile104, Leu120, Arg122, Val126, and Leu174 according to Figure 3A, wherein the root mean square deviation of the backbone atoms between said at least 8 amino acid residues and said human Pim-1 kinase amino acid residues which are identical is not greater than about 2.0 Å;

(iii) a set of amino acid residues comprising at least 12 amino acid residues which are identical to human Pim-1 kinase amino acid residues Leu43, Leu44, Gly45, Ser46, Gly47, Phe49, Gly50, Ser51, Val52, Tyr53, Ser54, Val64, Ala65, Ile66, Lys67, Ile104, Arg105, Leu118, Ile119, Leu120, Glu121, Arg122, Pro123, Glu124, Val126, Gln127, Asp128, Asp131, Glu171, Asn172, Ile173, Leu174, Ile175, Lys183, Leu184, Ile185 and Asp186 according to Figure 1A, 2A or 3A, wherein the root mean square deviation of the backbone atoms between said at least 12 amino acid residues and said human Pim-1 kinase amino acid residues is not greater than about 2.0 Å; and

(iv) a set of amino acid residues that are identical to human Pim-1 kinase amino acid residues according to Figure 1A, 2A or 3A, wherein the root mean square deviation between said set of amino acid residues and said human Pim-1 kinase amino acid residues is not more than about 3.0 Å;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine-readable data and a means for generating three-dimensional structural information of said binding pocket or protein; and

(d) output hardware coupled to said central processing unit for outputting three-dimensional structural information of said binding pocket or protein, or information produced using said three-dimensional structural information of said binding pocket or protein.

18. The computer according to claim 17, wherein the binding pocket is produced by homology modeling of the structure coordinates of said human Pim-1 kinase amino acid residues according to Figure 1A, 2A, or 3A.

19. The computer according to claim 17, wherein said means for generating three-dimensional structural information is provided by means for generating a three-dimensional graphical representation of said binding pocket or protein.

20. The computer according to claim 17, wherein said output hardware is a display terminal, a printer, CD or DVD recorder, ZIP™ or JAZ™ drive, a disk drive, or other machine-readable data storage device.

21. A method of using a computer for selecting an orientation of a chemical entity that interacts favorably with a binding pocket or protein selected from the group consisting of:

(i) a set of amino acid residues which are identical to human Pim-1 kinase amino acid residues Phe49, Ala65, Val126, and Leu174 according to Figure 1A, 2A or 3A, wherein the root mean square deviation of the backbone atoms between said amino acid residues and said human Pim-1 kinase amino acid residues which are identical is not greater than about 2.0 Å;

(ii) a set of amino acid residues comprising at least 8 amino acid residues which are identical to human Pim-1 kinase amino acid residues Leu44, Gly45, Phe49, Val52, Ala65, Lys67, Ile104, Leu120, Arg122, Val126, and Leu174 according to Figure 3A, wherein the root mean square deviation of the backbone atoms between said at least 8 amino acid residues and said human Pim-1 kinase amino acid residues which are identical is not greater than about 2.0 Å;

(iii) a set of amino acid residues comprising at least 12 amino acid residues which are identical to human Pim-1 kinase amino acid residues Leu43, Leu44, Gly45, Ser46, Gly47, Phe49, Gly50, Ser51, Val52, Tyr53, Ser54, Val64, Ala65, Ile66, Lys67, Ile104, Arg105, Leu118, Ile119, Leu120, Glu121,

Arg122, Pro123, Glu124, Val126, Gln127, Asp128, Asp131, Glu171, Asn172, Ile173, Leu174, Ile175, Lys183, Leu184, Ile185 and Asp186 according to Figure 1A, 2A or 3A, wherein the root mean square deviation of the backbone atoms between said at least 12 amino acid residues and said human Pim-1 kinase amino acid residues is not greater than about 2.0 Å; and

(iv) a set of amino acid residues that are identical to human Pim-1 kinase amino acid residues according to Figure 1A, 2A or 3A, wherein the root mean square deviation between said set of amino acid residues and said human Pim-1 kinase amino acid residues is not more than about 3.0 Å;

said method comprising the steps of:

(a) providing the structure coordinates of said binding pocket, or protein on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) employing computational means to dock a first chemical entity in the binding pocket or protein;

(c) quantifying the association between said chemical entity and all or part of the binding pocket or protein for different orientations of the chemical entity; and

(d) based on said quantified association.

22. The method according to claim 21, further comprising generating a three-dimensional graphical representation of the binding pocket or protein prior to step (b).

23. The method according to claim 21, wherein energy minimization, molecular dynamics simulations, or rigid-body minimizations are performed simultaneously with or following step (b).

24. The method according to claim 21, further comprising the steps of:

(e) repeating steps (b) through (d) with a second chemical entity; and

(f) selecting at least one of said first or second chemical entity that interacts more favorably with said binding pocket or protein based on said quantified association of said first or second chemical entity.

25. A method of using a computer for selecting an orientation of a chemical entity with a favorable shape complementarity in a binding pocket selected from the group consisting of:

(i) a set of amino acid residues which are identical to human Pim-1 kinase amino acid residues Phe49, Ala65, Val126, and Leu174 according to Figure 1A, 2A or 3A, wherein the root mean square deviation of the backbone atoms between said amino acid residues and said human Pim-1 kinase amino acid residues which are identical is not greater than about 2.0 Å;

(ii) a set of amino acid residues comprising at least 8 amino acid residues which are identical to human Pim-1 kinase amino acid residues Leu44, Gly45, Phe49, Val52, Ala65, Lys67, Ile104, Leu120, Arg122, Val126, and Leu174 according to Figure 3A, wherein the root mean square deviation of the backbone atoms between said at least 8 amino acid residues and said human Pim-1 kinase amino acid residues which are identical is not greater than about 2.0 Å; and

(iii) a set of amino acid residues comprising at least 12 amino acid residues which are identical to human Pim-1 kinase amino acid residues Leu43, Leu44, Gly45, Ser46, Gly47, Phe49, Gly50, Ser51, Val52, Tyr53, Ser54, Val64, Ala65, Ile66, Lys67, Ile104, Arg105, Leu118, Ile119, Leu120, Glu121, Arg122, Pro123, Glu124, Val126, Gln127, Asp128, Asp131, Glu171, Asn172, Ile173, Leu174, Ile175, Lys183, Leu184, Ile185 and Asp186 according to Figure 1A, 2A or 3A, wherein the root mean square deviation of the backbone atoms between said at least 12 amino acid residues and said human Pim-1 kinase amino acid residues is not greater than about 2.0 Å;

said method comprising the steps of:

(a) providing the structure coordinates of said binding pocket and all or part of the ligand bound therein on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) employing computational means to dock a first chemical entity in the binding pocket;

(c) quantitating the contact score of said chemical entity in different orientations; and

(d) selecting an orientation with the highest contact score.

26. The method according to claim 25, further comprising generating a three-dimensional graphical representation of the binding pocket and all or part of the ligand bound therein prior to step (b).

27. The method according to claim 25, further comprising the steps of:

(e) repeating steps (b) through (d) with a second chemical entity; and

(f) selecting at least one of said first or second chemical entity that has a higher contact score based on said quantitated contact score of said first or second chemical entity.

28. A method for identifying a candidate inhibitor of a molecule or molecular complex comprising a binding pocket or protein selected from the group consisting of:

(i) a set of amino acid residues which are identical to human Pim-1 kinase amino acid residues Phe49, Ala65, Val126, and Leu174 according to Figure 1A, 2A or 3A, wherein the root mean square deviation of the

backbone atoms between said amino acid residues and said human Pim-1 kinase amino acid residues which are identical is not greater than about 2.0 Å;

(ii) a set of amino acid residues comprising at least 8 amino acid residues which are identical to human Pim-1 kinase amino acid residues Leu44, Gly45, Phe49, Val52, Ala65, Lys67, Ile104, Leu120, Arg122, Val126, and Leu174 according to Figure 3A, wherein the root mean square deviation of the backbone atoms between said at least 8 amino acid residues and said human Pim-1 kinase amino acid residues which are identical is not greater than about 2.0 Å;

(iii) a set of amino acid residues comprising at least 12 amino acid residues which are identical to human Pim-1 kinase amino acid residues Leu43, Leu44, Gly45, Ser46, Gly47, Phe49, Gly50, Ser51, Val52, Tyr53, Ser54, Val64, Ala65, Ile66, Lys67, Ile104, Arg105, Leu118, Ile119, Leu120, Glu121, Arg122, Pro123, Glu124, Val126, Gln127, Asp128, Asp131, Glu171, Asn172, Ile173, Leu174, Ile175, Lys183, Leu184, Ile185 and Asp186 according to Figure 1A, 2A or 3A, wherein the root mean square deviation of the backbone atoms between said at least 12 amino acid residues and said human Pim-1 kinase amino acid residues is not greater than about 2.0 Å; and

(iv) a set of amino acid residues that are identical to human Pim-1 kinase amino acid residues according to Figure 1A, 2A or 3A, wherein the root mean square deviation between said set of amino acid residues and said human Pim-1 kinase amino acid residues is not more than about 3.0 Å;

comprising the steps of:

(a) using a three-dimensional structure of the binding pocket or protein to design, select or optimize a plurality of chemical entities;

(b) contacting each chemical entity with the molecule or the molecular complex;

(c) monitoring the inhibition to the catalytic activity of the molecule or molecular complex by each chemical entity; and

(d) selecting a chemical entity based on the inhibitory effect of the chemical entity on the catalytic activity of the molecule or molecular complex.

29. A method of designing a compound or complex that interacts with a binding pocket or protein selected from the group consisting of:

(i) a set of amino acid residues which are identical to human Pim-1 kinase amino acid residues Phe49, Ala65, Val126, and Leu174 according to Figure 1A, 2A or 3A, wherein the root mean square deviation of the backbone atoms between said amino acid residues and said human Pim-1 kinase amino acid residues which are identical is not greater than about 2.0 Å;

(ii) a set of amino acid residues comprising at least 8 amino acid residues which are identical to human Pim-1 kinase amino acid residues Leu44, Gly45, Phe49, Val52, Ala65, Lys67, Ile104, Leu120, Arg122, Val126, and Leu174 according to Figure 3A, wherein the root mean square deviation of the backbone atoms between said at least 8 amino acid residues and said human Pim-1 kinase amino acid residues which are identical is not greater than about 2.0 Å;

(iii) a set of amino acid residues comprising at least 12 amino acid residues which are identical to human Pim-1 kinase amino acid residues Leu43, Leu44, Gly45, Ser46, Gly47, Phe49, Gly50, Ser51, Val52, Tyr53, Ser54, Val64, Ala65, Ile66, Lys67, Ile104, Arg105, Leu118, Ile119, Leu120, Glu121, Arg122, Pro123, Glu124, Val126, Gln127, Asp128, Asp131, Glu171, Asn172, Ile173, Leu174, Ile175, Lys183, Leu184, Ile185 and Asp186 according to Figure 1A, 2A or 3A, wherein the root mean square deviation of the backbone atoms between said at least 12 amino acid residues and said human Pim-1 kinase amino acid residues is not greater than about 2.0 Å; and

(iv) a set of amino acid residues that are identical to human Pim-1 kinase amino acid residues according to Figure 1A, 2A or 3A, wherein the root mean square deviation between said set of amino acid residues and said human Pim-1 kinase amino acid residues is not more than about 3.0 Å;

comprising the steps of:

(a) providing the structure coordinates of said binding pocket or protein on a computer comprising the means for generating three-dimensional structural information from said structure coordinates;

(b) using the computer to dock a first chemical entity in part of the binding pocket or protein;

(c) docking at least a second chemical entity in another part of the binding pocket or protein;

(d) quantifying the association between the first or second chemical entity and part of the binding pocket or protein;

(e) repeating steps (b) to (d) with another first and second chemical entity, selecting a first and a second chemical entity based on said quantified association of all of said first and second chemical entity;

(f) optionally, visually inspecting the relationship of the first and second chemical entity to each other in relation to the binding pocket or protein on a computer screen using the three-dimensional graphical representation of the binding pocket or protein and said first and second chemical entity; and

(g) assembling the first and second chemical entity into a compound or complex that interacts with said binding pocket or protein by model building.

30. A method of utilizing molecular replacement to obtain structural information about a molecule or a molecular complex of unknown structure, wherein the molecule is sufficiently homologous to Pim-1 protein, comprising the steps of:

(a) crystallizing said molecule or molecular complex;

(b) generating X-ray diffraction data from said crystallized molecule or molecular complex; and

(c) applying at least a portion of the structure coordinates set forth in Figure 1A, 2A or 3A or homology model thereof to the X-ray diffraction data to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown; and

(d) generating a structural model of the molecule or molecular complex from the three-dimensional electron density map.

31. The method according to claim 30, wherein the molecule is selected from the group consisting of a Pim-1 protein and a Pim-1 protein homologue.

32. The method according to claim 30, wherein the molecular complex is selected from the group consisting of a Pim-1 protein complex and a Pim-1 homologue complex.

FIGURE 1A-1

ATOM	Type	Resid	#	X	Y	Z	Occ	B	
ATOM	1	CB	PRO A	33	-33.171	25.235	14.378	1.00	95.79	A C
ATOM	2	CG	PRO A	33	-33.277	26.076	15.657	1.00	96.01	A C
ATOM	3	C	PRO A	33	-31.733	26.730	12.964	1.00	95.96	A C
ATOM	4	O	PRO A	33	-32.747	27.406	12.773	1.00	96.06	A O
ATOM	5	N	PRO A	33	-30.986	25.884	15.170	1.00	95.87	A N
ATOM	6	CD	PRO A	33	-31.899	25.933	16.328	1.00	95.61	A C
ATOM	7	CA	PRO A	33	-31.750	25.555	13.940	1.00	96.01	A C
ATOM	8	N	LEU A	34	-30.575	26.963	12.350	1.00	95.36	A N
ATOM	9	CA	LEU A	34	-30.409	28.059	11.403	1.00	94.72	A C
ATOM	10	CB	LEU A	34	-29.085	27.904	10.636	1.00	94.44	A C
ATOM	11	CG	LEU A	34	-28.870	26.728	9.681	1.00	94.36	A C
ATOM	12	CD1	LEU A	34	-29.575	26.989	8.362	1.00	94.44	A C
ATOM	13	CD2	LEU A	34	-27.385	26.552	9.431	1.00	95.00	A C
ATOM	14	C	LEU A	34	-31.574	28.151	10.425	1.00	94.42	A C
ATOM	15	O	LEU A	34	-31.961	29.244	10.009	1.00	94.14	A O
ATOM	16	N	GLU A	35	-32.133	26.999	10.068	1.00	94.17	A N
ATOM	17	CA	GLU A	35	-33.256	26.944	9.138	1.00	93.91	A C
ATOM	18	CB	GLU A	35	-33.519	25.495	8.704	1.00	94.02	A C
ATOM	19	CG	GLU A	35	-32.270	24.714	8.310	1.00	94.85	A C
ATOM	20	CD	GLU A	35	-31.586	24.054	9.499	1.00	95.64	A C
ATOM	21	OE1	GLU A	35	-31.674	24.601	10.619	1.00	96.81	A O
ATOM	22	OE2	GLU A	35	-30.949	22.994	9.312	1.00	95.28	A O
ATOM	23	C	GLU A	35	-34.501	27.512	9.810	1.00	93.24	A C
ATOM	24	O	GLU A	35	-35.502	26.819	9.963	1.00	93.80	A O
ATOM	25	N	SER A	36	-34.433	28.775	10.215	1.00	92.32	A N
ATOM	26	CA	SER A	36	-35.557	29.421	10.880	1.00	90.93	A C
ATOM	27	CB	SER A	36	-35.897	28.674	12.173	1.00	91.28	A C
ATOM	28	OG	SER A	36	-36.968	29.301	12.856	1.00	90.93	A O
ATOM	29	C	SER A	36	-35.274	30.886	11.203	1.00	89.99	A C
ATOM	30	O	SER A	36	-36.172	31.729	11.137	1.00	89.75	A O
ATOM	31	N	GLN A	37	-34.027	31.189	11.554	1.00	88.38	A N
ATOM	32	CA	GLN A	37	-33.649	32.556	11.896	1.00	86.71	A C
ATOM	33	CB	GLN A	37	-32.488	32.545	12.885	1.00	87.32	A C
ATOM	34	CG	GLN A	37	-32.639	31.520	13.984	1.00	89.05	A C
ATOM	35	CD	GLN A	37	-31.403	31.418	14.847	1.00	90.11	A C
ATOM	36	OE1	GLN A	37	-31.234	30.455	15.597	1.00	91.48	A O
ATOM	37	NE2	GLN A	37	-30.531	32.416	14.751	1.00	90.30	A N
ATOM	38	C	GLN A	37	-33.245	33.334	10.652	1.00	84.86	A C
ATOM	39	O	GLN A	37	-33.080	34.553	10.696	1.00	85.24	A O
ATOM	40	N	TYR A	38	-33.093	32.623	9.541	1.00	82.50	A N
ATOM	41	CA	TYR A	38	-32.701	33.242	8.284	1.00	80.74	A C
ATOM	42	CB	TYR A	38	-31.224	32.952	7.994	1.00	78.99	A C
ATOM	43	CG	TYR A	38	-30.285	33.439	9.066	1.00	76.51	A C
ATOM	44	CD1	TYR A	38	-29.932	34.779	9.147	1.00	75.93	A C
ATOM	45	CE1	TYR A	38	-29.111	35.246	10.164	1.00	76.28	A C
ATOM	46	CD2	TYR A	38	-29.788	32.568	10.031	1.00	76.07	A C
ATOM	47	CE2	TYR A	38	-28.966	33.024	11.055	1.00	75.92	A C
ATOM	48	CZ	TYR A	38	-28.634	34.365	11.116	1.00	75.79	A C
ATOM	49	OH	TYR A	38	-27.845	34.836	12.140	1.00	76.01	A O
ATOM	50	C	TYR A	38	-33.542	32.689	7.147	1.00	80.41	A C
ATOM	51	O	TYR A	38	-33.943	31.527	7.173	1.00	80.41	A O
ATOM	52	N	GLN A	39	-33.820	33.525	6.153	1.00	79.80	A N
ATOM	53	CA	GLN A	39	-34.577	33.071	5.000	1.00	79.22	A C
ATOM	54	CB	GLN A	39	-35.858	33.890	4.813	1.00	80.28	A C

FIGURE 1A-2

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ATOM    55  CG  GLN A  39   -35.654  35.343   4.454  1.00 82.63   A C
ATOM    56  CD  GLN A  39   -36.950  36.021   4.039  1.00 84.05   A C
ATOM    57  OE1 GLN A  39   -36.952  37.182   3.625  1.00 84.23   A O
ATOM    58  NE2 GLN A  39   -38.061  35.295   4.148  1.00 84.07   A N
ATOM    59  C   GLN A  39   -33.667  33.193   3.784  1.00 77.93   A C
ATOM    60  O   GLN A  39   -33.318  34.294   3.352  1.00 78.00   A O
ATOM    61  N   VAL A  40   -33.271  32.042   3.252  1.00 76.24   A N
ATOM    62  CA  VAL A  40   -32.381  31.971   2.104  1.00 74.70   A C
ATOM    63  CB  VAL A  40   -32.055  30.508   1.765  1.00 75.22   A C
ATOM    64  CG1 VAL A  40   -31.516  29.802   3.000  1.00 74.95   A C
ATOM    65  CG2 VAL A  40   -33.303  29.804   1.254  1.00 76.59   A C
ATOM    66  C   VAL A  40   -32.933  32.645   0.854  1.00 73.04   A C
ATOM    67  O   VAL A  40   -34.141  32.693   0.639  1.00 73.08   A O
ATOM    68  N   GLY A  41   -32.026  33.160   0.032  1.00 71.25   A N
ATOM    69  CA  GLY A  41   -32.410  33.822  -1.197  1.00 68.73   A C
ATOM    70  C   GLY A  41   -31.636  33.245  -2.364  1.00 68.18   A C
ATOM    71  O   GLY A  41   -31.334  32.051  -2.374  1.00 67.47   A O
ATOM    72  N   PRO A  42   -31.296  34.067  -3.368  1.00 67.99   A N
ATOM    73  CD  PRO A  42   -31.718  35.470  -3.528  1.00 67.53   A C
ATOM    74  CA  PRO A  42   -30.547  33.613  -4.547  1.00 67.67   A C
ATOM    75  CB  PRO A  42   -30.735  34.762  -5.537  1.00 67.52   A C
ATOM    76  CG  PRO A  42   -30.812  35.955  -4.639  1.00 68.20   A C
ATOM    77  C   PRO A  42   -29.072  33.298  -4.295  1.00 66.70   A C
ATOM    78  O   PRO A  42   -28.484  33.747  -3.314  1.00 67.00   A O
ATOM    79  N   LEU A  43   -28.488  32.524  -5.202  1.00 65.71   A N
ATOM    80  CA  LEU A  43   -27.089  32.130  -5.118  1.00 66.09   A C
ATOM    81  CB  LEU A  43   -26.876  30.871  -5.975  1.00 66.00   A C
ATOM    82  CG  LEU A  43   -25.613  30.003  -5.928  1.00 66.51   A C
ATOM    83  CD1 LEU A  43   -25.813  28.827  -6.872  1.00 65.72   A C
ATOM    84  CD2 LEU A  43   -24.378  30.793  -6.337  1.00 67.19   A C
ATOM    85  C   LEU A  43   -26.204  33.282  -5.613  1.00 65.99   A C
ATOM    86  O   LEU A  43   -26.157  33.573  -6.809  1.00 67.02   A O
ATOM    87  N   LEU A  44   -25.511  33.943  -4.692  1.00 65.53   A N
ATOM    88  CA  LEU A  44   -24.636  35.055  -5.057  1.00 65.40   A C
ATOM    89  CB  LEU A  44   -24.092  35.737  -3.800  1.00 63.99   A C
ATOM    90  CG  LEU A  44   -25.116  36.388  -2.869  1.00 63.39   A C
ATOM    91  CD1 LEU A  44   -24.410  36.923  -1.645  1.00 63.37   A C
ATOM    92  CD2 LEU A  44   -25.839  37.506  -3.589  1.00 61.72   A C
ATOM    93  C   LEU A  44   -23.474  34.573  -5.922  1.00 65.59   A C
ATOM    94  O   LEU A  44   -23.259  35.070  -7.028  1.00 65.06   A O
ATOM    95  N   GLY A  45   -22.730  33.601  -5.410  1.00 66.90   A N
ATOM    96  CA  GLY A  45   -21.601  33.060  -6.145  1.00 68.47   A C
ATOM    97  C   GLY A  45   -21.186  31.694  -5.629  1.00 69.54   A C
ATOM    98  O   GLY A  45   -21.803  31.147  -4.711  1.00 69.30   A O
ATOM    99  N   SER A  46   -20.132  31.141  -6.215  1.00 70.26   A N
ATOM   100  CA  SER A  46   -19.638  29.831  -5.814  1.00 71.62   A C
ATOM   101  CB  SER A  46   -20.623  28.744  -6.249  1.00 72.10   A C
ATOM   102  OG  SER A  46   -20.001  27.470  -6.275  1.00 71.47   A O
ATOM   103  C   SER A  46   -18.277  29.550  -6.427  1.00 72.62   A C
ATOM   104  O   SER A  46   -17.892  30.168  -7.419  1.00 72.99   A O
ATOM   105  N   GLY A  47   -17.548  28.611  -5.837  1.00 73.55   A N
ATOM   106  CA  GLY A  47   -16.244  28.276  -6.372  1.00 75.31   A C
ATOM   107  C   GLY A  47   -15.290  27.686  -5.356  1.00 76.33   A C
ATOM   108  O   GLY A  47   -15.704  26.963  -4.447  1.00 76.20   A O
ATOM   109  N   GLY A  48   -14.006  28.000  -5.519  1.00 76.88   A N
ATOM   110  CA  GLY A  48   -12.986  27.499  -4.616  1.00 77.35   A C
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FIGURE 1A-3

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ATOM  111  C   GLY A  48  -13.061  28.118  -3.235  1.00 77.55  A C
ATOM  112  O   GLY A  48  -12.070  28.630  -2.715  1.00 79.09  A O
ATOM  113  N   PHE A  49  -14.251  28.082  -2.649  1.00 77.06  A N
ATOM  114  CA  PHE A  49  -14.487  28.616  -1.317  1.00 75.61  A C
ATOM  115  CB  PHE A  49  -14.386  30.149  -1.307  1.00 77.67  A C
ATOM  116  CG  PHE A  49  -15.301  30.837  -2.283  1.00 79.76  A C
ATOM  117  CD1 PHE A  49  -14.981  30.898  -3.637  1.00 80.26  A C
ATOM  118  CD2 PHE A  49  -16.482  31.433  -1.844  1.00 80.97  A C
ATOM  119  CE1 PHE A  49  -15.824  31.543  -4.544  1.00 80.88  A C
ATOM  120  CE2 PHE A  49  -17.334  32.080  -2.740  1.00 81.73  A C
ATOM  121  CZ  PHE A  49  -17.004  32.136  -4.093  1.00 82.35  A C
ATOM  122  C   PHE A  49  -15.864  28.175  -0.833  1.00 73.32  A C
ATOM  123  O   PHE A  49  -16.200  28.335   0.340  1.00 74.09  A O
ATOM  124  N   GLY A  50  -16.653  27.612  -1.745  1.00 69.75  A N
ATOM  125  CA  GLY A  50  -17.980  27.138  -1.388  1.00 65.40  A C
ATOM  126  C   GLY A  50  -19.106  27.710  -2.229  1.00 61.30  A C
ATOM  127  O   GLY A  50  -18.917  28.056  -3.398  1.00 61.23  A O
ATOM  128  N   SER A  51  -20.285  27.799  -1.624  1.00 57.06  A N
ATOM  129  CA  SER A  51  -21.463  28.331  -2.286  1.00 52.09  A C
ATOM  130  CB  SER A  51  -22.453  27.204  -2.557  1.00 52.18  A C
ATOM  131  OG  SER A  51  -21.804  26.117  -3.195  1.00 49.97  A O
ATOM  132  C   SER A  51  -22.054  29.345  -1.323  1.00 50.22  A C
ATOM  133  O   SER A  51  -22.288  29.036  -0.156  1.00 50.12  A O
ATOM  134  N   VAL A  52  -22.284  30.557  -1.809  1.00 49.24  A N
ATOM  135  CA  VAL A  52  -22.806  31.634  -0.976  1.00 48.54  A C
ATOM  136  CB  VAL A  52  -21.866  32.852  -1.031  1.00 48.09  A C
ATOM  137  CG1 VAL A  52  -22.407  33.970  -0.156  1.00 48.06  A C
ATOM  138  CG2 VAL A  52  -20.464  32.445  -0.598  1.00 45.71  A C
ATOM  139  C   VAL A  52  -24.198  32.073  -1.410  1.00 49.32  A C
ATOM  140  O   VAL A  52  -24.426  32.375  -2.583  1.00 48.66  A O
ATOM  141  N   TYR A  53  -25.123  32.126  -0.458  1.00 49.14  A N
ATOM  142  CA  TYR A  53  -26.491  32.514  -0.765  1.00 49.88  A C
ATOM  143  CB  TYR A  53  -27.482  31.430  -0.315  1.00 48.29  A C
ATOM  144  CG  TYR A  53  -27.331  30.083  -0.992  1.00 47.09  A C
ATOM  145  CD1 TYR A  53  -26.359  29.179  -0.575  1.00 46.21  A C
ATOM  146  CE1 TYR A  53  -26.225  27.933  -1.183  1.00 45.74  A C
ATOM  147  CD2 TYR A  53  -28.172  29.709  -2.042  1.00 45.58  A C
ATOM  148  CE2 TYR A  53  -28.051  28.467  -2.659  1.00 45.74  A C
ATOM  149  CZ  TYR A  53  -27.073  27.582  -2.224  1.00 46.68  A C
ATOM  150  OH  TYR A  53  -26.939  26.349  -2.820  1.00 45.40  A O
ATOM  151  C   TYR A  53  -26.878  33.812  -0.088  1.00 52.07  A C
ATOM  152  O   TYR A  53  -26.504  34.056   1.060  1.00 53.08  A O
ATOM  153  N   SER A  54  -27.633  34.644  -0.799  1.00 53.36  A N
ATOM  154  CA  SER A  54  -28.100  35.896  -0.229  1.00 54.66  A C
ATOM  155  CB  SER A  54  -28.737  36.776  -1.303  1.00 56.56  A C
ATOM  156  OG  SER A  54  -29.258  37.970  -0.738  1.00 57.39  A O
ATOM  157  C   SER A  54  -29.151  35.471   0.771  1.00 55.54  A C
ATOM  158  O   SER A  54  -29.838  34.482   0.552  1.00 57.11  A O
ATOM  159  N   GLY A  55  -29.277  36.197   1.872  1.00 56.69  A N
ATOM  160  CA  GLY A  55  -30.265  35.818   2.862  1.00 57.74  A C
ATOM  161  C   GLY A  55  -30.683  36.976   3.736  1.00 59.97  A C
ATOM  162  O   GLY A  55  -30.129  38.072   3.642  1.00 60.66  A O
ATOM  163  N   ILE A  56  -31.666  36.732   4.592  1.00 61.87  A N
ATOM  164  CA  ILE A  56  -32.166  37.756   5.493  1.00 63.96  A C
ATOM  165  CB  ILE A  56  -33.486  38.334   4.972  1.00 64.00  A C
ATOM  166  CG2 ILE A  56  -34.115  39.224   6.024  1.00 64.54  A C
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FIGURE 1A-4

```
ATOM  167  CG1 ILE A  56  -33.225  39.092   3.670  1.00 64.20  A C
ATOM  168  CD1 ILE A  56  -34.462  39.645   3.018  1.00 66.40  A C
ATOM  169  C   ILE A  56  -32.378  37.166   6.876  1.00 65.41  A C
ATOM  170  O   ILE A  56  -32.829  36.029   7.017  1.00 65.71  A O
ATOM  171  N   ARG A  57  -32.043  37.942   7.897  1.00 67.56  A N
ATOM  172  CA  ARG A  57  -32.184  37.490   9.274  1.00 70.49  A C
ATOM  173  CB  ARG A  57  -31.038  38.047  10.124  1.00 70.48  A C
ATOM  174  CG  ARG A  57  -31.095  37.653  11.587  1.00 70.93  A C
ATOM  175  CD  ARG A  57  -30.515  38.758  12.450  1.00 72.66  A C
ATOM  176  NE  ARG A  57  -29.132  38.528  12.854  1.00 72.93  A N
ATOM  177  CZ  ARG A  57  -28.350  39.469  13.375  1.00 73.59  A C
ATOM  178  NH1 ARG A  57  -28.815  40.702  13.543  1.00 72.48  A N
ATOM  179  NH2 ARG A  57  -27.111  39.176  13.747  1.00 73.98  A N
ATOM  180  C   ARG A  57  -33.518  37.921   9.873  1.00 72.46  A C
ATOM  181  O   ARG A  57  -33.658  39.052  10.341  1.00 72.86  A O
ATOM  182  N   VAL A  58  -34.500  37.025   9.847  1.00 74.77  A N
ATOM  183  CA  VAL A  58  -35.809  37.329  10.416  1.00 76.58  A C
ATOM  184  CB  VAL A  58  -36.801  36.153  10.249  1.00 77.57  A C
ATOM  185  CG1 VAL A  58  -37.645  36.357   8.992  1.00 78.73  A C
ATOM  186  CG2 VAL A  58  -36.043  34.834  10.171  1.00 76.99  A C
ATOM  187  C   VAL A  58  -35.620  37.605  11.899  1.00 77.54  A C
ATOM  188  O   VAL A  58  -35.488  36.679  12.702  1.00 77.82  A O
ATOM  189  N   SER A  59  -35.594  38.887  12.248  1.00 77.64  A N
ATOM  190  CA  SER A  59  -35.403  39.329  13.625  1.00 77.81  A C
ATOM  191  CB  SER A  59  -34.213  38.602  14.265  1.00 77.71  A C
ATOM  192  OG  SER A  59  -33.988  39.046  15.592  1.00 77.00  A O
ATOM  193  C   SER A  59  -35.118  40.821  13.561  1.00 77.93  A C
ATOM  194  O   SER A  59  -35.281  41.550  14.541  1.00 78.40  A O
ATOM  195  N   ASP A  60  -34.680  41.255  12.385  1.00 77.28  A N
ATOM  196  CA  ASP A  60  -34.363  42.651  12.121  1.00 76.50  A C
ATOM  197  CB  ASP A  60  -33.076  43.063  12.842  1.00 76.36  A C
ATOM  198  CG  ASP A  60  -31.985  42.015  12.740  1.00 77.05  A C
ATOM  199  OD1 ASP A  60  -31.788  41.464  11.639  1.00 78.35  A O
ATOM  200  OD2 ASP A  60  -31.317  41.747  13.760  1.00 77.02  A O
ATOM  201  C   ASP A  60  -34.191  42.798  10.619  1.00 75.75  A C
ATOM  202  O   ASP A  60  -33.706  43.815  10.130  1.00 75.85  A O
ATOM  203  N   ASN A  61  -34.600  41.757   9.898  1.00 75.12  A N
ATOM  204  CA  ASN A  61  -34.509  41.718   8.443  1.00 73.88  A C
ATOM  205  CB  ASN A  61  -35.595  42.606   7.834  1.00 75.02  A C
ATOM  206  CG  ASN A  61  -36.973  41.979   7.936  1.00 76.42  A C
ATOM  207  OD1 ASN A  61  -37.350  41.136   7.116  1.00 77.77  A O
ATOM  208  ND2 ASN A  61  -37.723  42.368   8.958  1.00 77.92  A N
ATOM  209  C   ASN A  61  -33.134  42.127   7.935  1.00 71.79  A C
ATOM  210  O   ASN A  61  -32.995  42.643   6.826  1.00 72.31  A O
ATOM  211  N   LEU A  62  -32.119  41.884   8.757  1.00 68.70  A N
ATOM  212  CA  LEU A  62  -30.742  42.211   8.415  1.00 65.30  A C
ATOM  213  CB  LEU A  62  -29.824  41.876   9.582  1.00 64.78  A C
ATOM  214  CG  LEU A  62  -28.330  42.078   9.353  1.00 64.66  A C
ATOM  215  CD1 LEU A  62  -28.040  43.563   9.191  1.00 62.89  A C
ATOM  216  CD2 LEU A  62  -27.555  41.501  10.536  1.00 64.09  A C
ATOM  217  C   LEU A  62  -30.284  41.422   7.201  1.00 63.14  A C
ATOM  218  O   LEU A  62  -30.404  40.195   7.170  1.00 63.45  A O
ATOM  219  N   PRO A  63  -29.759  42.115   6.180  1.00 60.40  A N
ATOM  220  CD  PRO A  63  -29.628  43.577   6.051  1.00 59.26  A C
ATOM  221  CA  PRO A  63  -29.284  41.435   4.972  1.00 58.16  A C
ATOM  222  CB  PRO A  63  -29.052  42.587   3.996  1.00 58.42  A C
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FIGURE 1A-5

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ATOM  223  CG  PRO A  63  -28.656  43.712   4.903  1.00 59.05  A C
ATOM  224  C   PRO A  63  -28.001  40.666   5.282  1.00 56.23  A C
ATOM  225  O   PRO A  63  -27.017  41.251   5.740  1.00 55.75  A O
ATOM  226  N   VAL A  64  -28.015  39.358   5.046  1.00 54.00  A N
ATOM  227  CA  VAL A  64  -26.841  38.534   5.318  1.00 52.00  A C
ATOM  228  CB  VAL A  64  -27.078  37.591   6.512  1.00 51.82  A C
ATOM  229  CG1 VAL A  64  -27.487  38.390   7.737  1.00 50.74  A C
ATOM  230  CG2 VAL A  64  -28.135  36.558   6.152  1.00 50.25  A C
ATOM  231  C   VAL A  64  -26.412  37.667   4.141  1.00 51.00  A C
ATOM  232  O   VAL A  64  -27.080  37.607   3.107  1.00 51.41  A O
ATOM  233  N   ALA A  65  -25.280  36.994   4.319  1.00 49.23  A N
ATOM  234  CA  ALA A  65  -24.738  36.099   3.313  1.00 46.30  A C
ATOM  235  CB  ALA A  65  -23.413  36.625   2.788  1.00 46.31  A C
ATOM  236  C   ALA A  65  -24.539  34.774   4.011  1.00 44.81  A C
ATOM  237  O   ALA A  65  -23.964  34.717   5.095  1.00 44.20  A O
ATOM  238  N   ILE A  66  -25.032  33.711   3.391  1.00 44.29  A N
ATOM  239  CA  ILE A  66  -24.926  32.374   3.954  1.00 43.19  A C
ATOM  240  CB  ILE A  66  -26.319  31.714   4.025  1.00 42.65  A C
ATOM  241  CG2 ILE A  66  -26.231  30.355   4.694  1.00 42.79  A C
ATOM  242  CG1 ILE A  66  -27.267  32.623   4.814  1.00 43.20  A C
ATOM  243  CD1 ILE A  66  -28.670  32.087   4.931  1.00 44.11  A C
ATOM  244  C   ILE A  66  -23.979  31.541   3.098  1.00 43.39  A C
ATOM  245  O   ILE A  66  -24.244  31.277   1.921  1.00 44.79  A O
ATOM  246  N   LYS A  67  -22.872  31.130   3.704  1.00 42.07  A N
ATOM  247  CA  LYS A  67  -21.859  30.361   3.006  1.00 41.68  A C
ATOM  248  CB  LYS A  67  -20.500  31.030   3.210  1.00 42.24  A C
ATOM  249  CG  LYS A  67  -19.351  30.375   2.476  1.00 44.06  A C
ATOM  250  CD  LYS A  67  -18.080  31.203   2.646  1.00 45.96  A C
ATOM  251  CE  LYS A  67  -16.903  30.597   1.901  1.00 46.87  A C
ATOM  252  NZ  LYS A  67  -15.705  31.473   1.985  1.00 49.41  A N
ATOM  253  C   LYS A  67  -21.806  28.912   3.472  1.00 42.16  A C
ATOM  254  O   LYS A  67  -21.769  28.629   4.672  1.00 41.99  A O
ATOM  255  N   HIS A  68  -21.798  27.998   2.509  1.00 42.59  A N
ATOM  256  CA  HIS A  68  -21.755  26.575   2.802  1.00 42.14  A C
ATOM  257  CB  HIS A  68  -22.875  25.849   2.062  1.00 41.00  A C
ATOM  258  CG  HIS A  68  -24.244  26.290   2.463  1.00 38.32  A C
ATOM  259  CD2 HIS A  68  -24.972  27.373   2.100  1.00 38.85  A C
ATOM  260  ND1 HIS A  68  -25.000  25.614   3.394  1.00 38.50  A N
ATOM  261  CE1 HIS A  68  -26.135  26.263   3.593  1.00 39.33  A C
ATOM  262  NE2 HIS A  68  -26.142  27.336   2.820  1.00 38.96  A N
ATOM  263  C   HIS A  68  -20.423  26.006   2.372  1.00 43.43  A C
ATOM  264  O   HIS A  68  -19.941  26.297   1.279  1.00 43.19  A O
ATOM  265  N   VAL A  69  -19.836  25.196   3.244  1.00 46.68  A N
ATOM  266  CA  VAL A  69  -18.555  24.555   2.977  1.00 49.69  A C
ATOM  267  CB  VAL A  69  -17.421  25.213   3.793  1.00 49.99  A C
ATOM  268  CG1 VAL A  69  -16.101  24.524   3.509  1.00 50.19  A C
ATOM  269  CG2 VAL A  69  -17.322  26.687   3.443  1.00 52.29  A C
ATOM  270  C   VAL A  69  -18.658  23.089   3.373  1.00 51.34  A C
ATOM  271  O   VAL A  69  -19.041  22.772   4.494  1.00 52.67  A O
ATOM  272  N   GLU A  70  -18.334  22.196   2.446  1.00 54.79  A N
ATOM  273  CA  GLU A  70  -18.391  20.763   2.717  1.00 58.41  A C
ATOM  274  CB  GLU A  70  -18.412  19.965   1.409  1.00 61.38  A C
ATOM  275  CG  GLU A  70  -19.667  20.157   0.575  1.00 65.88  A C
ATOM  276  CD  GLU A  70  -19.536  19.565  -0.819  1.00 68.99  A C
ATOM  277  OE1 GLU A  70  -18.526  19.869  -1.498  1.00 70.26  A O
ATOM  278  OE2 GLU A  70  -20.444  18.809  -1.236  1.00 69.77  A O
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FIGURE 1A-6

```
ATOM  279  C   GLU A  70  -17.180  20.352   3.533  1.00 59.11  A C
ATOM  280  O   GLU A  70  -16.052  20.737   3.224  1.00 58.68  A O
ATOM  281  N   LYS A  71  -17.415  19.562   4.573  1.00 60.45  A N
ATOM  282  CA  LYS A  71  -16.331  19.104   5.425  1.00 62.00  A C
ATOM  283  CB  LYS A  71  -16.877  18.161   6.491  1.00 60.54  A C
ATOM  284  CG  LYS A  71  -17.881  18.811   7.413  1.00 59.86  A C
ATOM  285  CD  LYS A  71  -18.300  17.853   8.509  1.00 60.97  A C
ATOM  286  CE  LYS A  71  -19.300  18.502   9.443  1.00 60.49  A C
ATOM  287  NZ  LYS A  71  -19.671  17.596  10.555  1.00 61.13  A N
ATOM  288  C   LYS A  71  -15.208  18.417   4.647  1.00 63.87  A C
ATOM  289  O   LYS A  71  -14.032  18.664   4.894  1.00 64.19  A O
ATOM  290  N   ASP A  72  -15.566  17.567   3.695  1.00 67.14  A N
ATOM  291  CA  ASP A  72  -14.558  16.856   2.923  1.00 70.66  A C
ATOM  292  CB  ASP A  72  -15.233  15.857   1.980  1.00 72.66  A C
ATOM  293  CG  ASP A  72  -16.146  14.888   2.719  1.00 75.38  A C
ATOM  294  OD1 ASP A  72  -15.731  14.377   3.784  1.00 75.65  A O
ATOM  295  OD2 ASP A  72  -17.273  14.632   2.237  1.00 77.05  A O
ATOM  296  C   ASP A  72  -13.643  17.778   2.129  1.00 72.22  A C
ATOM  297  O   ASP A  72  -12.528  17.398   1.777  1.00 71.95  A O
ATOM  298  N   ARG A  73  -14.105  18.999   1.875  1.00 74.78  A N
ATOM  299  CA  ARG A  73  -13.340  19.968   1.093  1.00 76.54  A C
ATOM  300  CB  ARG A  73  -14.299  20.838   0.277  1.00 78.28  A C
ATOM  301  CG  ARG A  73  -14.905  20.127  -0.918  1.00 81.43  A C
ATOM  302  CD  ARG A  73  -13.862  19.943  -2.006  1.00 84.51  A C
ATOM  303  NE  ARG A  73  -14.303  19.027  -3.055  1.00 86.97  A N
ATOM  304  CZ  ARG A  73  -13.611  18.775  -4.163  1.00 87.93  A C
ATOM  305  NH1 ARG A  73  -12.444  19.377  -4.370  1.00 87.91  A N
ATOM  306  NH2 ARG A  73  -14.081  17.918  -5.060  1.00 87.98  A N
ATOM  307  C   ARG A  73  -12.366  20.873   1.839  1.00 76.84  A C
ATOM  308  O   ARG A  73  -11.678  21.677   1.211  1.00 76.94  A O
ATOM  309  N   ILE A  74  -12.290  20.759   3.161  1.00 77.20  A N
ATOM  310  CA  ILE A  74  -11.368  21.614   3.904  1.00 78.24  A C
ATOM  311  CB  ILE A  74  -12.090  22.367   5.042  1.00 78.32  A C
ATOM  312  CG2 ILE A  74  -13.512  22.694   4.625  1.00 77.74  A C
ATOM  313  CG1 ILE A  74  -12.128  21.513   6.305  1.00 78.49  A C
ATOM  314  CD1 ILE A  74  -12.697  22.235   7.491  1.00 79.28  A C
ATOM  315  C   ILE A  74  -10.207  20.821   4.495  1.00 78.46  A C
ATOM  316  O   ILE A  74  -10.369  19.659   4.864  1.00 78.38  A O
ATOM  317  N   SER A  75   -9.039  21.455   4.588  1.00 79.23  A N
ATOM  318  CA  SER A  75   -7.857  20.792   5.133  1.00 79.94  A C
ATOM  319  CB  SER A  75   -6.721  20.807   4.108  1.00 81.39  A C
ATOM  320  OG  SER A  75   -5.612  20.051   4.572  1.00 83.58  A O
ATOM  321  C   SER A  75   -7.351  21.384   6.451  1.00 79.30  A C
ATOM  322  O   SER A  75   -6.617  20.724   7.185  1.00 79.45  A O
ATOM  323  N   ASP A  76   -7.731  22.622   6.752  1.00 78.39  A N
ATOM  324  CA  ASP A  76   -7.297  23.249   7.994  1.00 77.49  A C
ATOM  325  CB  ASP A  76   -6.724  24.636   7.730  1.00 79.74  A C
ATOM  326  CG  ASP A  76   -5.231  24.612   7.526  1.00 81.86  A C
ATOM  327  OD1 ASP A  76   -4.562  23.810   8.212  1.00 83.60  A O
ATOM  328  OD2 ASP A  76   -4.727  25.400   6.698  1.00 83.41  A O
ATOM  329  C   ASP A  76   -8.401  23.366   9.024  1.00 75.88  A C
ATOM  330  O   ASP A  76   -9.496  23.827   8.715  1.00 75.57  A O
ATOM  331  N   TRP A  77   -8.102  22.950  10.252  1.00 74.22  A N
ATOM  332  CA  TRP A  77   -9.070  23.015  11.342  1.00 72.93  A C
ATOM  333  CB  TRP A  77   -9.619  21.624  11.673  1.00 71.28  A C
ATOM  334  CG  TRP A  77  -10.092  20.810  10.504  1.00 69.10  A C
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FIGURE 1A-7

```
ATOM  335  CD2 TRP A  77  -11.445  20.436  10.206  1.00 67.81  A C
ATOM  336  CE2 TRP A  77  -11.406  19.598   9.068  1.00 67.85  A C
ATOM  337  CE3 TRP A  77  -12.685  20.724  10.793  1.00 66.60  A C
ATOM  338  CD1 TRP A  77   -9.314  20.209   9.556  1.00 69.04  A C
ATOM  339  NE1 TRP A  77  -10.095  19.477   8.692  1.00 68.15  A N
ATOM  340  CZ2 TRP A  77  -12.560  19.045   8.504  1.00 67.97  A C
ATOM  341  CZ3 TRP A  77  -13.836  20.172  10.231  1.00 66.90  A C
ATOM  342  CH2 TRP A  77  -13.763  19.342   9.098  1.00 67.73  A C
ATOM  343  C   TRP A  77   -8.412  23.588  12.592  1.00 72.97  A C
ATOM  344  O   TRP A  77   -7.196  23.510  12.747  1.00 73.39  A O
ATOM  345  N   GLY A  78   -9.225  24.155  13.478  1.00 73.08  A N
ATOM  346  CA  GLY A  78   -8.717  24.730  14.713  1.00 74.25  A C
ATOM  347  C   GLY A  78   -9.766  24.639  15.808  1.00 75.69  A C
ATOM  348  O   GLY A  78  -10.734  23.889  15.676  1.00 76.37  A O
ATOM  349  N   ALA A  79   -9.588  25.394  16.888  1.00 76.51  A N
ATOM  350  CA  ALA A  79  -10.548  25.371  17.988  1.00 77.48  A C
ATOM  351  CB  ALA A  79  -10.252  24.193  18.912  1.00 77.36  A C
ATOM  352  C   ALA A  79  -10.519  26.678  18.777  1.00 78.43  A C
ATOM  353  O   ALA A  79   -9.616  27.495  18.507  1.00 78.47  A O
ATOM  354  OXT ALA A  79  -11.392  26.871  19.657  1.00 79.13  A O
ATOM  355  CB  THR A  84  -15.748  22.664  19.224  1.00 78.82  A C
ATOM  356  OG1 THR A  84  -15.876  23.702  18.246  1.00 79.61  A O
ATOM  357  CG2 THR A  84  -16.311  23.166  20.541  1.00 78.53  A C
ATOM  358  C   THR A  84  -13.568  22.442  18.040  1.00 77.34  A C
ATOM  359  O   THR A  84  -13.094  23.523  17.691  1.00 77.45  A O
ATOM  360  N   THR A  84  -13.586  23.179  20.378  1.00 78.70  A N
ATOM  361  CA  THR A  84  -14.263  22.291  19.387  1.00 78.49  A C
ATOM  362  N   ARG A  85  -13.520  21.356  17.282  1.00 75.82  A N
ATOM  363  CA  ARG A  85  -12.852  21.367  15.993  1.00 74.31  A C
ATOM  364  CB  ARG A  85  -12.414  19.942  15.640  1.00 76.05  A C
ATOM  365  CG  ARG A  85  -11.573  19.852  14.388  1.00 79.31  A C
ATOM  366  CD  ARG A  85  -11.155  18.422  14.095  1.00 81.12  A C
ATOM  367  NE  ARG A  85  -11.106  18.179  12.656  1.00 83.33  A N
ATOM  368  CZ  ARG A  85  -10.770  17.022  12.096  1.00 84.52  A C
ATOM  369  NH1 ARG A  85  -10.441  15.983  12.853  1.00 85.40  A N
ATOM  370  NH2 ARG A  85  -10.780  16.897  10.775  1.00 85.29  A N
ATOM  371  C   ARG A  85  -13.695  21.962  14.862  1.00 72.15  A C
ATOM  372  O   ARG A  85  -14.582  21.304  14.315  1.00 72.01  A O
ATOM  373  N   VAL A  86  -13.409  23.215  14.516  1.00 68.71  A N
ATOM  374  CA  VAL A  86  -14.127  23.906  13.447  1.00 63.49  A C
ATOM  375  CB  VAL A  86  -14.759  25.227  13.947  1.00 63.27  A C
ATOM  376  CG1 VAL A  86  -15.681  24.955  15.120  1.00 62.03  A C
ATOM  377  CG2 VAL A  86  -13.671  26.207  14.345  1.00 61.83  A C
ATOM  378  C   VAL A  86  -13.141  24.245  12.337  1.00 60.75  A C
ATOM  379  O   VAL A  86  -11.930  24.201  12.546  1.00 59.70  A O
ATOM  380  N   PRO A  87  -13.642  24.567  11.132  1.00 58.54  A N
ATOM  381  CD  PRO A  87  -15.013  24.449  10.607  1.00 56.89  A C
ATOM  382  CA  PRO A  87  -12.699  24.905  10.060  1.00 55.85  A C
ATOM  383  CB  PRO A  87  -13.603  25.068   8.829  1.00 56.33  A C
ATOM  384  CG  PRO A  87  -14.958  25.345   9.408  1.00 57.40  A C
ATOM  385  C   PRO A  87  -11.896  26.167  10.390  1.00 53.78  A C
ATOM  386  O   PRO A  87  -12.390  27.074  11.059  1.00 52.93  A O
ATOM  387  N   MET A  88  -10.651  26.209   9.926  1.00 52.50  A N
ATOM  388  CA  MET A  88   -9.774  27.343  10.181  1.00 51.02  A C
ATOM  389  CB  MET A  88   -8.480  27.200   9.374  1.00 52.08  A C
ATOM  390  CG  MET A  88   -7.449  28.292   9.643  1.00 52.96  A C
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FIGURE 1A-8

```
ATOM  391  SD  MET A  88     -6.951  28.375  11.390  1.00 56.48  A S
ATOM  392  CE  MET A  88     -6.239  26.751  11.614  1.00 53.36  A C
ATOM  393  C   MET A  88    -10.444  28.667   9.837  1.00 49.04  A C
ATOM  394  O   MET A  88    -10.293  29.657  10.563  1.00 48.61  A O
ATOM  395  N   GLU A  89    -11.184  28.681   8.732  1.00 46.30  A N
ATOM  396  CA  GLU A  89    -11.860  29.895   8.295  1.00 44.67  A C
ATOM  397  CB  GLU A  89    -12.740  29.600   7.072  1.00 43.93  A C
ATOM  398  CG  GLU A  89    -13.417  30.830   6.463  1.00 43.39  A C
ATOM  399  CD  GLU A  89    -14.135  30.534   5.147  1.00 43.18  A C
ATOM  400  OE1 GLU A  89    -14.762  31.462   4.584  1.00 41.19  A O
ATOM  401  OE2 GLU A  89    -14.065  29.379   4.671  1.00 42.68  A O
ATOM  402  C   GLU A  89    -12.695  30.503   9.424  1.00 44.34  A C
ATOM  403  O   GLU A  89    -12.728  31.723   9.593  1.00 44.17  A O
ATOM  404  N   VAL A  90    -13.357  29.657  10.208  1.00 43.60  A N
ATOM  405  CA  VAL A  90    -14.187  30.143  11.305  1.00 42.76  A C
ATOM  406  CB  VAL A  90    -15.080  29.016  11.884  1.00 43.47  A C
ATOM  407  CG1 VAL A  90    -15.919  29.556  13.038  1.00 42.68  A C
ATOM  408  CG2 VAL A  90    -15.982  28.457  10.792  1.00 43.73  A C
ATOM  409  C   VAL A  90    -13.323  30.717  12.420  1.00 42.37  A C
ATOM  410  O   VAL A  90    -13.644  31.765  12.977  1.00 41.69  A O
ATOM  411  N   VAL A  91    -12.231  30.029  12.746  1.00 41.33  A N
ATOM  412  CA  VAL A  91    -11.329  30.496  13.791  1.00 40.55  A C
ATOM  413  CB  VAL A  91    -10.117  29.553  13.957  1.00 41.17  A C
ATOM  414  CG1 VAL A  91     -9.078  30.188  14.883  1.00 39.48  A C
ATOM  415  CG2 VAL A  91    -10.573  28.221  14.519  1.00 40.77  A C
ATOM  416  C   VAL A  91    -10.814  31.873  13.410  1.00 40.09  A C
ATOM  417  O   VAL A  91    -10.809  32.799  14.221  1.00 40.51  A O
ATOM  418  N   LEU A  92    -10.379  31.995  12.163  1.00 39.67  A N
ATOM  419  CA  LEU A  92     -9.860  33.252  11.651  1.00 39.56  A C
ATOM  420  CB  LEU A  92     -9.362  33.048  10.215  1.00 39.08  A C
ATOM  421  CG  LEU A  92     -7.876  32.702  10.021  1.00 39.30  A C
ATOM  422  CD1 LEU A  92     -7.305  31.980  11.229  1.00 36.80  A C
ATOM  423  CD2 LEU A  92     -7.717  31.879   8.765  1.00 38.72  A C
ATOM  424  C   LEU A  92    -10.907  34.366  11.716  1.00 40.30  A C
ATOM  425  O   LEU A  92    -10.676  35.398  12.341  1.00 41.08  A O
ATOM  426  N   LEU A  93    -12.059  34.159  11.088  1.00 40.47  A N
ATOM  427  CA  LEU A  93    -13.110  35.171  11.104  1.00 40.51  A C
ATOM  428  CB  LEU A  93    -14.368  34.658  10.396  1.00 39.99  A C
ATOM  429  CG  LEU A  93    -14.338  34.629   8.868  1.00 40.61  A C
ATOM  430  CD1 LEU A  93    -15.549  33.874   8.337  1.00 38.70  A C
ATOM  431  CD2 LEU A  93    -14.303  36.060   8.342  1.00 39.55  A C
ATOM  432  C   LEU A  93    -13.484  35.626  12.507  1.00 40.89  A C
ATOM  433  O   LEU A  93    -13.718  36.805  12.745  1.00 39.95  A O
ATOM  434  N   LYS A  94    -13.535  34.692  13.444  1.00 43.26  A N
ATOM  435  CA  LYS A  94    -13.918  35.033  14.807  1.00 45.18  A C
ATOM  436  CB  LYS A  94    -14.073  33.759  15.633  1.00 47.58  A C
ATOM  437  CG  LYS A  94    -14.698  33.985  16.988  1.00 52.58  A C
ATOM  438  CD  LYS A  94    -15.086  32.654  17.624  1.00 57.84  A C
ATOM  439  CE  LYS A  94    -16.143  31.947  16.795  1.00 59.20  A C
ATOM  440  NZ  LYS A  94    -17.343  32.827  16.619  1.00 63.56  A N
ATOM  441  C   LYS A  94    -12.937  35.985  15.478  1.00 44.81  A C
ATOM  442  O   LYS A  94    -13.345  36.964  16.101  1.00 44.58  A O
ATOM  443  N   LYS A  95    -11.646  35.701  15.347  1.00 44.91  A N
ATOM  444  CA  LYS A  95    -10.621  36.549  15.941  1.00 45.68  A C
ATOM  445  CB  LYS A  95     -9.238  35.917  15.755  1.00 44.91  A C
ATOM  446  CG  LYS A  95     -9.102  34.503  16.309  1.00 45.25  A C
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FIGURE 1A-9

```
ATOM  447  CD  LYS A  95      -7.688  33.964  16.136  1.00 45.59   A C
ATOM  448  CE  LYS A  95      -6.715  34.682  17.042  1.00 48.56   A C
ATOM  449  NZ  LYS A  95      -5.323  34.232  16.780  1.00 51.97   A N
ATOM  450  C   LYS A  95     -10.610  37.936  15.303  1.00 46.74   A C
ATOM  451  O   LYS A  95     -10.144  38.907  15.907  1.00 46.99   A O
ATOM  452  N   VAL A  96     -11.149  38.026  14.091  1.00 46.87   A N
ATOM  453  CA  VAL A  96     -11.150  39.270  13.334  1.00 47.06   A C
ATOM  454  CB  VAL A  96     -10.584  38.986  11.916  1.00 46.03   A C
ATOM  455  CG1 VAL A  96     -11.663  39.178  10.851  1.00 43.98   A C
ATOM  456  CG2 VAL A  96      -9.378  39.848  11.660  1.00 46.77   A C
ATOM  457  C   VAL A  96     -12.495  39.996  13.204  1.00 48.72   A C
ATOM  458  O   VAL A  96     -12.543  41.121  12.714  1.00 48.75   A O
ATOM  459  N   SER A  97     -13.573  39.366  13.661  1.00 51.04   A N
ATOM  460  CA  SER A  97     -14.921  39.926  13.537  1.00 53.89   A C
ATOM  461  CB  SER A  97     -15.906  38.810  13.146  1.00 51.97   A C
ATOM  462  OG  SER A  97     -15.689  38.352  11.832  1.00 49.56   A O
ATOM  463  C   SER A  97     -15.522  40.709  14.706  1.00 56.73   A C
ATOM  464  O   SER A  97     -16.736  40.920  14.743  1.00 57.74   A O
ATOM  465  N   SER A  98     -14.714  41.145  15.661  1.00 60.23   A N
ATOM  466  CA  SER A  98     -15.283  41.896  16.777  1.00 64.28   A C
ATOM  467  CB  SER A  98     -14.809  41.290  18.105  1.00 65.24   A C
ATOM  468  OG  SER A  98     -13.632  40.526  17.911  1.00 68.23   A O
ATOM  469  C   SER A  98     -14.910  43.368  16.652  1.00 65.62   A C
ATOM  470  O   SER A  98     -13.775  43.714  16.316  1.00 66.05   A O
ATOM  471  N   GLY A  99     -15.895  44.221  16.901  1.00 66.83   A N
ATOM  472  CA  GLY A  99     -15.691  45.650  16.795  1.00 67.84   A C
ATOM  473  C   GLY A  99     -15.933  46.039  15.347  1.00 69.04   A C
ATOM  474  O   GLY A  99     -16.444  45.238  14.572  1.00 69.02   A O
ATOM  475  N   PHE A 100     -15.569  47.258  14.972  1.00 70.14   A N
ATOM  476  CA  PHE A 100     -15.745  47.709  13.606  1.00 69.84   A C
ATOM  477  CB  PHE A 100     -16.132  49.180  13.599  1.00 72.32   A C
ATOM  478  CG  PHE A 100     -17.460  49.438  14.199  1.00 75.41   A C
ATOM  479  CD1 PHE A 100     -17.593  50.280  15.300  1.00 76.16   A C
ATOM  480  CD2 PHE A 100     -18.588  48.814  13.678  1.00 76.39   A C
ATOM  481  CE1 PHE A 100     -18.841  50.493  15.870  1.00 77.15   A C
ATOM  482  CE2 PHE A 100     -19.842  49.018  14.237  1.00 76.59   A C
ATOM  483  CZ  PHE A 100     -19.967  49.859  15.337  1.00 76.86   A C
ATOM  484  C   PHE A 100     -14.461  47.517  12.841  1.00 67.97   A C
ATOM  485  O   PHE A 100     -13.393  47.438  13.441  1.00 67.88   A O
ATOM  486  N   SER A 101     -14.564  47.460  11.517  1.00 64.98   A N
ATOM  487  CA  SER A 101     -13.382  47.278  10.694  1.00 63.38   A C
ATOM  488  CB  SER A 101     -12.537  46.138  11.285  1.00 65.08   A C
ATOM  489  OG  SER A 101     -12.028  45.266  10.299  1.00 69.88   A O
ATOM  490  C   SER A 101     -13.706  47.026   9.218  1.00 60.01   A C
ATOM  491  O   SER A 101     -14.877  46.938   8.828  1.00 59.63   A O
ATOM  492  N   GLY A 102     -12.651  46.926   8.408  1.00 55.91   A N
ATOM  493  CA  GLY A 102     -12.796  46.702   6.975  1.00 50.67   A C
ATOM  494  C   GLY A 102     -12.839  45.257   6.478  1.00 47.46   A C
ATOM  495  O   GLY A 102     -12.438  44.971   5.350  1.00 47.26   A O
ATOM  496  N   VAL A 103     -13.333  44.350   7.319  1.00 44.81   A N
ATOM  497  CA  VAL A 103     -13.459  42.926   6.988  1.00 43.28   A C
ATOM  498  CB  VAL A 103     -12.613  42.022   7.917  1.00 42.21   A C
ATOM  499  CG1 VAL A 103     -11.176  42.492   7.943  1.00 42.53   A C
ATOM  500  CG2 VAL A 103     -13.187  42.031   9.314  1.00 41.51   A C
ATOM  501  C   VAL A 103     -14.891  42.468   7.165  1.00 42.77   A C
ATOM  502  O   VAL A 103     -15.514  42.834   8.158  1.00 43.41   A O
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FIGURE 1A-10

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ATOM  503  N   ILE A 104  -15.411  41.642   6.258  1.00 42.52  A N
ATOM  504  CA  ILE A 104  -16.777  41.159   6.428  1.00 42.38  A C
ATOM  505  CB  ILE A 104  -17.214  40.245   5.270  1.00 42.83  A C
ATOM  506  CG2 ILE A 104  -18.516  39.523   5.604  1.00 42.74  A C
ATOM  507  CG1 ILE A 104  -17.431  41.084   4.022  1.00 43.20  A C
ATOM  508  CD1 ILE A 104  -18.488  42.151   4.169  1.00 42.68  A C
ATOM  509  C   ILE A 104  -16.821  40.373   7.736  1.00 42.71  A C
ATOM  510  O   ILE A 104  -16.102  39.393   7.908  1.00 42.44  A O
ATOM  511  N   ARG A 105  -17.680  40.811   8.649  1.00 43.68  A N
ATOM  512  CA  ARG A 105  -17.817  40.177   9.953  1.00 46.89  A C
ATOM  513  CB  ARG A 105  -18.453  41.158  10.945  1.00 49.91  A C
ATOM  514  CG  ARG A 105  -17.541  42.300  11.369  1.00 55.20  A C
ATOM  515  CD  ARG A 105  -17.602  42.521  12.880  1.00 60.74  A C
ATOM  516  NE  ARG A 105  -18.868  43.097  13.323  1.00 65.39  A N
ATOM  517  CZ  ARG A 105  -19.241  44.346  13.064  1.00 68.49  A C
ATOM  518  NH1 ARG A 105  -18.439  45.149  12.369  1.00 70.24  A N
ATOM  519  NH2 ARG A 105  -20.423  44.786  13.477  1.00 69.79  A N
ATOM  520  C   ARG A 105  -18.619  38.881   9.955  1.00 46.16  A C
ATOM  521  O   ARG A 105  -19.619  38.760   9.253  1.00 46.76  A O
ATOM  522  N   LEU A 106  -18.167  37.914  10.747  1.00 44.71  A N
ATOM  523  CA  LEU A 106  -18.860  36.639  10.873  1.00 43.74  A C
ATOM  524  CB  LEU A 106  -17.892  35.533  11.272  1.00 43.55  A C
ATOM  525  CG  LEU A 106  -18.565  34.193  11.564  1.00 43.99  A C
ATOM  526  CD1 LEU A 106  -18.983  33.524  10.259  1.00 42.91  A C
ATOM  527  CD2 LEU A 106  -17.595  33.316  12.327  1.00 44.73  A C
ATOM  528  C   LEU A 106  -19.895  36.810  11.972  1.00 43.63  A C
ATOM  529  O   LEU A 106  -19.548  36.943  13.143  1.00 43.12  A O
ATOM  530  N   LEU A 107  -21.163  36.799  11.586  1.00 44.28  A N
ATOM  531  CA  LEU A 107  -22.261  36.984  12.521  1.00 45.34  A C
ATOM  532  CB  LEU A 107  -23.496  37.458  11.755  1.00 44.38  A C
ATOM  533  CG  LEU A 107  -23.750  38.965  11.635  1.00 42.69  A C
ATOM  534  CD1 LEU A 107  -22.488  39.750  11.857  1.00 43.28  A C
ATOM  535  CD2 LEU A 107  -24.350  39.265  10.273  1.00 45.10  A C
ATOM  536  C   LEU A 107  -22.606  35.755  13.343  1.00 46.52  A C
ATOM  537  O   LEU A 107  -22.998  35.876  14.497  1.00 45.38  A O
ATOM  538  N   ASP A 108  -22.454  34.576  12.748  1.00 48.77  A N
ATOM  539  CA  ASP A 108  -22.771  33.321  13.429  1.00 49.73  A C
ATOM  540  CB  ASP A 108  -24.282  33.254  13.695  1.00 52.96  A C
ATOM  541  CG  ASP A 108  -24.684  32.118  14.633  1.00 54.08  A C
ATOM  542  OD1 ASP A 108  -25.896  32.017  14.934  1.00 56.93  A O
ATOM  543  OD2 ASP A 108  -23.814  31.334  15.069  1.00 53.91  A O
ATOM  544  C   ASP A 108  -22.356  32.170  12.520  1.00 49.88  A C
ATOM  545  O   ASP A 108  -21.912  32.392  11.391  1.00 50.52  A O
ATOM  546  N   TRP A 109  -22.499  30.947  13.011  1.00 49.69  A N
ATOM  547  CA  TRP A 109  -22.156  29.769  12.232  1.00 51.14  A C
ATOM  548  CB  TRP A 109  -20.649  29.570  12.198  1.00 50.06  A C
ATOM  549  CG  TRP A 109  -20.066  29.339  13.544  1.00 50.48  A C
ATOM  550  CD2 TRP A 109  -19.750  28.076  14.131  1.00 50.62  A C
ATOM  551  CE2 TRP A 109  -19.214  28.332  15.410  1.00 50.70  A C
ATOM  552  CE3 TRP A 109  -19.867  26.747  13.700  1.00 51.80  A C
ATOM  553  CD1 TRP A 109  -19.729  30.284  14.462  1.00 50.14  A C
ATOM  554  NE1 TRP A 109  -19.212  29.690  15.586  1.00 50.64  A N
ATOM  555  CZ2 TRP A 109  -18.794  27.311  16.267  1.00 51.85  A C
ATOM  556  CZ3 TRP A 109  -19.449  25.726  14.555  1.00 52.57  A C
ATOM  557  CH2 TRP A 109  -18.917  26.018  15.825  1.00 51.75  A C
ATOM  558  C   TRP A 109  -22.804  28.520  12.821  1.00 53.01  A C
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FIGURE 1A-11

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ATOM   559  O   TRP A 109   -23.112  28.470  14.014  1.00 53.43   A O
ATOM   560  N   PHE A 110   -23.002  27.513  11.975  1.00 53.79   A N
ATOM   561  CA  PHE A 110   -23.611  26.264  12.404  1.00 54.18   A C
ATOM   562  CB  PHE A 110   -25.087  26.204  11.994  1.00 54.42   A C
ATOM   563  CG  PHE A 110   -25.903  27.361  12.493  1.00 55.23   A C
ATOM   564  CD1 PHE A 110   -25.954  28.550  11.779  1.00 54.45   A C
ATOM   565  CD2 PHE A 110   -26.609  27.268  13.689  1.00 56.39   A C
ATOM   566  CE1 PHE A 110   -26.693  29.629  12.245  1.00 56.25   A C
ATOM   567  CE2 PHE A 110   -27.352  28.344  14.164  1.00 57.19   A C
ATOM   568  CZ  PHE A 110   -27.394  29.527  13.438  1.00 56.67   A C
ATOM   569  C   PHE A 110   -22.888  25.096  11.782  1.00 53.44   A C
ATOM   570  O   PHE A 110   -22.248  25.233  10.742  1.00 53.55   A O
ATOM   571  N   GLU A 111   -22.987  23.945  12.433  1.00 54.58   A N
ATOM   572  CA  GLU A 111   -22.369  22.735  11.923  1.00 55.57   A C
ATOM   573  CB  GLU A 111   -21.493  22.076  12.989  1.00 56.61   A C
ATOM   574  CG  GLU A 111   -21.049  20.664  12.626  1.00 58.61   A C
ATOM   575  CD  GLU A 111   -19.950  20.149  13.533  1.00 61.24   A C
ATOM   576  OE1 GLU A 111   -19.963  20.496  14.736  1.00 62.28   A O
ATOM   577  OE2 GLU A 111   -19.079  19.391  13.048  1.00 62.31   A O
ATOM   578  C   GLU A 111   -23.475  21.778  11.493  1.00 55.24   A C
ATOM   579  O   GLU A 111   -24.520  21.683  12.139  1.00 54.84   A O
ATOM   580  N   ARG A 112   -23.241  21.089  10.385  1.00 54.19   A N
ATOM   581  CA  ARG A 112   -24.196  20.135   9.854  1.00 54.11   A C
ATOM   582  CB  ARG A 112   -24.784  20.637   8.539  1.00 51.40   A C
ATOM   583  CG  ARG A 112   -25.931  21.591   8.691  1.00 48.34   A C
ATOM   584  CD  ARG A 112   -26.275  22.141   7.337  1.00 47.18   A C
ATOM   585  NE  ARG A 112   -27.523  22.883   7.353  1.00 47.49   A N
ATOM   586  CZ  ARG A 112   -28.074  23.414   6.270  1.00 46.63   A C
ATOM   587  NH1 ARG A 112   -27.473  23.282   5.094  1.00 43.99   A N
ATOM   588  NH2 ARG A 112   -29.228  24.065   6.361  1.00 45.48   A N
ATOM   589  C   ARG A 112   -23.488  18.821   9.606  1.00 54.93   A C
ATOM   590  O   ARG A 112   -22.261  18.758   9.595  1.00 55.67   A O
ATOM   591  N   PRO A 113   -24.258  17.751   9.396  1.00 55.57   A N
ATOM   592  CD  PRO A 113   -25.731  17.689   9.324  1.00 56.50   A C
ATOM   593  CA  PRO A 113   -23.667  16.441   9.147  1.00 55.98   A C
ATOM   594  CB  PRO A 113   -24.802  15.691   8.463  1.00 57.21   A C
ATOM   595  CG  PRO A 113   -25.997  16.187   9.236  1.00 57.20   A C
ATOM   596  C   PRO A 113   -22.402  16.497   8.304  1.00 55.93   A C
ATOM   597  O   PRO A 113   -21.337  16.089   8.760  1.00 55.92   A O
ATOM   598  N   ASP A 114   -22.506  17.026   7.088  1.00 56.67   A N
ATOM   599  CA  ASP A 114   -21.343  17.089   6.206  1.00 57.08   A C
ATOM   600  CB  ASP A 114   -21.604  16.256   4.951  1.00 60.93   A C
ATOM   601  CG  ASP A 114   -21.820  14.787   5.261  1.00 64.77   A C
ATOM   602  OD1 ASP A 114   -22.920  14.439   5.748  1.00 66.56   A O
ATOM   603  OD2 ASP A 114   -20.883  13.986   5.022  1.00 65.83   A O
ATOM   604  C   ASP A 114   -20.853  18.474   5.779  1.00 55.31   A C
ATOM   605  O   ASP A 114   -20.155  18.603   4.770  1.00 55.47   A O
ATOM   606  N   SER A 115   -21.190  19.511   6.535  1.00 52.18   A N
ATOM   607  CA  SER A 115   -20.742  20.841   6.152  1.00 48.97   A C
ATOM   608  CB  SER A 115   -21.517  21.308   4.921  1.00 47.33   A C
ATOM   609  OG  SER A 115   -22.870  21.582   5.250  1.00 44.00   A O
ATOM   610  C   SER A 115   -20.919  21.862   7.261  1.00 47.68   A C
ATOM   611  O   SER A 115   -21.535  21.577   8.291  1.00 46.90   A O
ATOM   612  N   PHE A 116   -20.369  23.051   7.038  1.00 45.33   A N
ATOM   613  CA  PHE A 116   -20.499  24.148   7.988  1.00 44.49   A C
ATOM   614  CB  PHE A 116   -19.130  24.625   8.480  1.00 46.82   A C
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FIGURE 1A-12

```
ATOM   615  CG  PHE A 116  -18.515  23.743   9.527  1.00 48.10  A C
ATOM   616  CD1 PHE A 116  -17.701  22.680   9.169  1.00 48.55  A C
ATOM   617  CD2 PHE A 116  -18.762  23.977  10.876  1.00 49.05  A C
ATOM   618  CE1 PHE A 116  -17.140  21.865  10.142  1.00 50.25  A C
ATOM   619  CE2 PHE A 116  -18.207  23.169  11.856  1.00 48.64  A C
ATOM   620  CZ  PHE A 116  -17.397  22.113  11.491  1.00 49.41  A C
ATOM   621  C   PHE A 116  -21.208  25.296   7.289  1.00 42.69  A C
ATOM   622  O   PHE A 116  -21.015  25.517   6.095  1.00 42.96  A O
ATOM   623  N   VAL A 117  -22.028  26.023   8.033  1.00 39.96  A N
ATOM   624  CA  VAL A 117  -22.758  27.145   7.474  1.00 40.41  A C
ATOM   625  CB  VAL A 117  -24.286  26.940   7.640  1.00 40.95  A C
ATOM   626  CG1 VAL A 117  -25.053  28.158   7.137  1.00 39.29  A C
ATOM   627  CG2 VAL A 117  -24.712  25.704   6.870  1.00 41.63  A C
ATOM   628  C   VAL A 117  -22.316  28.428   8.177  1.00 40.88  A C
ATOM   629  O   VAL A 117  -22.380  28.536   9.406  1.00 39.39  A O
ATOM   630  N   LEU A 118  -21.859  29.396   7.393  1.00 41.45  A N
ATOM   631  CA  LEU A 118  -21.396  30.658   7.950  1.00 41.72  A C
ATOM   632  CB  LEU A 118  -20.007  30.996   7.400  1.00 42.61  A C
ATOM   633  CG  LEU A 118  -18.890  29.967   7.591  1.00 43.65  A C
ATOM   634  CD1 LEU A 118  -17.591  30.504   6.995  1.00 44.33  A C
ATOM   635  CD2 LEU A 118  -18.707  29.688   9.060  1.00 43.85  A C
ATOM   636  C   LEU A 118  -22.345  31.803   7.636  1.00 40.96  A C
ATOM   637  O   LEU A 118  -22.748  31.990   6.487  1.00 41.07  A O
ATOM   638  N   ILE A 119  -22.704  32.565   8.662  1.00 39.96  A N
ATOM   639  CA  ILE A 119  -23.584  33.707   8.481  1.00 40.59  A C
ATOM   640  CB  ILE A 119  -24.610  33.824   9.640  1.00 40.83  A C
ATOM   641  CG2 ILE A 119  -25.619  34.920   9.331  1.00 39.99  A C
ATOM   642  CG1 ILE A 119  -25.334  32.487   9.849  1.00 39.27  A C
ATOM   643  CD1 ILE A 119  -26.075  31.976   8.635  1.00 38.82  A C
ATOM   644  C   ILE A 119  -22.704  34.962   8.454  1.00 41.54  A C
ATOM   645  O   ILE A 119  -22.149  35.377   9.476  1.00 42.72  A O
ATOM   646  N   LEU A 120  -22.564  35.555   7.275  1.00 41.85  A N
ATOM   647  CA  LEU A 120  -21.748  36.750   7.124  1.00 41.21  A C
ATOM   648  CB  LEU A 120  -20.797  36.615   5.929  1.00 38.40  A C
ATOM   649  CG  LEU A 120  -19.605  35.658   5.919  1.00 37.07  A C
ATOM   650  CD1 LEU A 120  -18.926  35.677   7.276  1.00 36.81  A C
ATOM   651  CD2 LEU A 120  -20.055  34.272   5.560  1.00 38.22  A C
ATOM   652  C   LEU A 120  -22.609  37.974   6.892  1.00 41.91  A C
ATOM   653  O   LEU A 120  -23.762  37.856   6.496  1.00 43.29  A O
ATOM   654  N   GLU A 121  -22.035  39.147   7.137  1.00 43.65  A N
ATOM   655  CA  GLU A 121  -22.730  40.406   6.897  1.00 46.99  A C
ATOM   656  CB  GLU A 121  -21.873  41.608   7.321  1.00 46.59  A C
ATOM   657  CG  GLU A 121  -21.534  41.722   8.794  1.00 49.20  A C
ATOM   658  CD  GLU A 121  -20.804  43.029   9.116  1.00 52.40  A C
ATOM   659  OE1 GLU A 121  -19.729  43.271   8.525  1.00 52.33  A O
ATOM   660  OE2 GLU A 121  -21.306  43.815   9.957  1.00 53.64  A O
ATOM   661  C   GLU A 121  -22.900  40.489   5.384  1.00 48.53  A C
ATOM   662  O   GLU A 121  -22.247  39.750   4.639  1.00 49.12  A O
ATOM   663  N   ARG A 122  -23.775  41.375   4.925  1.00 49.24  A N
ATOM   664  CA  ARG A 122  -23.942  41.566   3.490  1.00 52.01  A C
ATOM   665  CB  ARG A 122  -25.018  40.653   2.895  1.00 52.86  A C
ATOM   666  CG  ARG A 122  -25.216  40.893   1.388  1.00 54.65  A C
ATOM   667  CD  ARG A 122  -26.173  39.892   0.755  1.00 56.31  A C
ATOM   668  NE  ARG A 122  -27.437  39.817   1.480  1.00 59.26  A N
ATOM   669  CZ  ARG A 122  -28.623  40.146   0.974  1.00 59.74  A C
ATOM   670  NH1 ARG A 122  -28.723  40.580  -0.276  1.00 60.61  A N
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FIGURE 1A-13

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ATOM   671  NH2 ARG A 122   -29.712  40.036   1.722  1.00 58.53   A N
ATOM   672  C   ARG A 122   -24.293  43.007   3.191  1.00 52.93   A C
ATOM   673  O   ARG A 122   -25.431  43.426   3.362  1.00 54.79   A O
ATOM   674  N   PRO A 123   -23.305  43.798   2.762  1.00 53.77   A N
ATOM   675  CD  PRO A 123   -21.867  43.491   2.627  1.00 54.28   A C
ATOM   676  CA  PRO A 123   -23.592  45.199   2.452  1.00 53.19   A C
ATOM   677  CB  PRO A 123   -22.202  45.826   2.376  1.00 54.38   A C
ATOM   678  CG  PRO A 123   -21.335  44.693   1.889  1.00 54.55   A C
ATOM   679  C   PRO A 123   -24.357  45.252   1.133  1.00 53.04   A C
ATOM   680  O   PRO A 123   -24.296  44.314   0.342  1.00 52.85   A O
ATOM   681  N   GLU A 124   -25.092  46.332   0.902  1.00 52.71   A N
ATOM   682  CA  GLU A 124   -25.863  46.459  -0.327  1.00 52.18   A C
ATOM   683  CB  GLU A 124   -27.176  45.674  -0.213  1.00 54.02   A C
ATOM   684  CG  GLU A 124   -27.390  44.639  -1.315  1.00 58.68   A C
ATOM   685  CD  GLU A 124   -26.796  43.269  -0.979  1.00 61.90   A C
ATOM   686  OE1 GLU A 124   -27.411  42.534  -0.172  1.00 63.67   A O
ATOM   687  OE2 GLU A 124   -25.718  42.925  -1.518  1.00 62.39   A O
ATOM   688  C   GLU A 124   -26.159  47.930  -0.578  1.00 49.74   A C
ATOM   689  O   GLU A 124   -26.609  48.637   0.318  1.00 49.58   A O
ATOM   690  N   PRO A 125   -25.908  48.411  -1.803  1.00 47.32   A N
ATOM   691  CD  PRO A 125   -25.955  49.841  -2.138  1.00 47.03   A C
ATOM   692  CA  PRO A 125   -25.364  47.641  -2.926  1.00 45.92   A C
ATOM   693  CB  PRO A 125   -25.570  48.566  -4.136  1.00 44.66   A C
ATOM   694  CG  PRO A 125   -26.267  49.796  -3.593  1.00 46.55   A C
ATOM   695  C   PRO A 125   -23.881  47.348  -2.724  1.00 44.00   A C
ATOM   696  O   PRO A 125   -23.222  48.003  -1.924  1.00 43.25   A O
ATOM   697  N   VAL A 126   -23.366  46.374  -3.467  1.00 42.34   A N
ATOM   698  CA  VAL A 126   -21.961  46.008  -3.393  1.00 41.41   A C
ATOM   699  CB  VAL A 126   -21.679  44.922  -2.326  1.00 41.07   A C
ATOM   700  CG1 VAL A 126   -22.010  45.441  -0.957  1.00 41.52   A C
ATOM   701  CG2 VAL A 126   -22.476  43.665  -2.636  1.00 40.26   A C
ATOM   702  C   VAL A 126   -21.471  45.454  -4.710  1.00 40.68   A C
ATOM   703  O   VAL A 126   -22.252  44.982  -5.533  1.00 40.93   A O
ATOM   704  N   GLN A 127   -20.158  45.513  -4.887  1.00 40.21   A N
ATOM   705  CA  GLN A 127   -19.507  44.984  -6.070  1.00 38.82   A C
ATOM   706  CB  GLN A 127   -19.505  46.009  -7.200  1.00 36.46   A C
ATOM   707  CG  GLN A 127   -19.217  45.385  -8.547  1.00 35.90   A C
ATOM   708  CD  GLN A 127   -19.135  46.404  -9.658  1.00 38.05   A C
ATOM   709  OE1 GLN A 127   -19.220  46.055 -10.837  1.00 38.97   A O
ATOM   710  NE2 GLN A 127   -18.957  47.672  -9.292  1.00 34.86   A N
ATOM   711  C   GLN A 127   -18.078  44.678  -5.655  1.00 38.98   A C
ATOM   712  O   GLN A 127   -17.470  45.462  -4.919  1.00 39.35   A O
ATOM   713  N   ASP A 128   -17.543  43.540  -6.099  1.00 37.62   A N
ATOM   714  CA  ASP A 128   -16.178  43.205  -5.744  1.00 36.16   A C
ATOM   715  CB  ASP A 128   -15.952  41.682  -5.795  1.00 37.07   A C
ATOM   716  CG  ASP A 128   -15.957  41.110  -7.203  1.00 39.81   A C
ATOM   717  OD1 ASP A 128   -16.424  39.957  -7.358  1.00 41.86   A O
ATOM   718  OD2 ASP A 128   -15.481  41.776  -8.149  1.00 42.24   A O
ATOM   719  C   ASP A 128   -15.236  43.981  -6.662  1.00 36.40   A C
ATOM   720  O   ASP A 128   -15.627  44.412  -7.752  1.00 35.70   A O
ATOM   721  N   LEU A 129   -14.007  44.186  -6.205  1.00 35.04   A N
ATOM   722  CA  LEU A 129   -13.035  44.951  -6.966  1.00 33.71   A C
ATOM   723  CB  LEU A 129   -11.720  45.056  -6.189  1.00 32.07   A C
ATOM   724  CG  LEU A 129   -11.108  46.444  -5.991  1.00 30.48   A C
ATOM   725  CD1 LEU A 129    -9.649  46.278  -5.585  1.00 26.97   A C
ATOM   726  CD2 LEU A 129   -11.221  47.273  -7.251  1.00 27.52   A C
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FIGURE 1A-14

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ATOM   727  C   LEU A 129  -12.766  44.368  -8.344  1.00 33.91  A C
ATOM   728  O   LEU A 129  -12.484  45.106  -9.287  1.00 33.12  A O
ATOM   729  N   PHE A 130  -12.834  43.048  -8.462  1.00 35.04  A N
ATOM   730  CA  PHE A 130  -12.588  42.413  -9.754  1.00 38.48  A C
ATOM   731  CB  PHE A 130  -12.668  40.890  -9.645  1.00 40.55  A C
ATOM   732  CG  PHE A 130  -12.443  40.181 -10.952  1.00 42.99  A C
ATOM   733  CD1 PHE A 130  -11.165  40.025 -11.460  1.00 44.18  A C
ATOM   734  CD2 PHE A 130  -13.521  39.710 -11.698  1.00 43.96  A C
ATOM   735  CE1 PHE A 130  -10.956  39.413 -12.693  1.00 45.48  A C
ATOM   736  CE2 PHE A 130  -13.324  39.095 -12.935  1.00 44.49  A C
ATOM   737  CZ  PHE A 130  -12.038  38.947 -13.433  1.00 44.67  A C
ATOM   738  C   PHE A 130  -13.608  42.893 -10.784  1.00 39.95  A C
ATOM   739  O   PHE A 130  -13.239  43.347 -11.865  1.00 40.62  A O
ATOM   740  N   ASP A 131  -14.891  42.790 -10.452  1.00 40.49  A N
ATOM   741  CA  ASP A 131  -15.931  43.239 -11.369  1.00 42.13  A C
ATOM   742  CB  ASP A 131  -17.316  42.882 -10.830  1.00 43.63  A C
ATOM   743  CG  ASP A 131  -17.556  41.392 -10.792  1.00 46.47  A C
ATOM   744  OD1 ASP A 131  -17.073  40.692 -11.713  1.00 46.94  A O
ATOM   745  OD2 ASP A 131  -18.237  40.923  -9.850  1.00 48.31  A O
ATOM   746  C   ASP A 131  -15.863  44.747 -11.606  1.00 42.03  A C
ATOM   747  O   ASP A 131  -16.100  45.226 -12.719  1.00 42.47  A O
ATOM   748  N   PHE A 132  -15.537  45.492 -10.555  1.00 41.20  A N
ATOM   749  CA  PHE A 132  -15.459  46.942 -10.649  1.00 40.96  A C
ATOM   750  CB  PHE A 132  -15.214  47.532  -9.259  1.00 40.11  A C
ATOM   751  CG  PHE A 132  -15.223  49.034  -9.217  1.00 40.24  A C
ATOM   752  CD1 PHE A 132  -14.075  49.760  -9.517  1.00 39.81  A C
ATOM   753  CD2 PHE A 132  -16.372  49.722  -8.841  1.00 39.07  A C
ATOM   754  CE1 PHE A 132  -14.067  51.157  -9.438  1.00 42.38  A C
ATOM   755  CE2 PHE A 132  -16.378  51.116  -8.759  1.00 40.58  A C
ATOM   756  CZ  PHE A 132  -15.219  51.836  -9.057  1.00 41.61  A C
ATOM   757  C   PHE A 132  -14.373  47.369 -11.623  1.00 42.28  A C
ATOM   758  O   PHE A 132  -14.592  48.249 -12.460  1.00 42.94  A O
ATOM   759  N   ILE A 133  -13.206  46.739 -11.529  1.00 42.38  A N
ATOM   760  CA  ILE A 133  -12.098  47.066 -12.419  1.00 42.65  A C
ATOM   761  CB  ILE A 133  -10.784  46.434 -11.907  1.00 41.75  A C
ATOM   762  CG2 ILE A 133   -9.701  46.523 -12.961  1.00 38.96  A C
ATOM   763  CG1 ILE A 133  -10.346  47.156 -10.630  1.00 42.25  A C
ATOM   764  CD1 ILE A 133   -9.208  46.487  -9.897  1.00 44.38  A C
ATOM   765  C   ILE A 133  -12.405  46.586 -13.835  1.00 43.75  A C
ATOM   766  O   ILE A 133  -12.109  47.269 -14.813  1.00 42.64  A O
ATOM   767  N   THR A 134  -13.012  45.411 -13.934  1.00 45.80  A N
ATOM   768  CA  THR A 134  -13.380  44.840 -15.222  1.00 47.23  A C
ATOM   769  CB  THR A 134  -14.023  43.441 -15.020  1.00 46.61  A C
ATOM   770  OG1 THR A 134  -13.025  42.525 -14.546  1.00 46.27  A O
ATOM   771  CG2 THR A 134  -14.625  42.915 -16.321  1.00 45.06  A C
ATOM   772  C   THR A 134  -14.345  45.757 -15.991  1.00 48.73  A C
ATOM   773  O   THR A 134  -14.287  45.832 -17.216  1.00 49.59  A O
ATOM   774  N   GLU A 135  -15.221  46.460 -15.277  1.00 50.03  A N
ATOM   775  CA  GLU A 135  -16.181  47.362 -15.921  1.00 52.24  A C
ATOM   776  CB  GLU A 135  -17.454  47.502 -15.080  1.00 52.45  A C
ATOM   777  CG  GLU A 135  -18.316  46.262 -15.007  1.00 54.34  A C
ATOM   778  CD  GLU A 135  -19.550  46.482 -14.161  1.00 55.38  A C
ATOM   779  OE1 GLU A 135  -20.291  45.498 -13.929  1.00 56.41  A O
ATOM   780  OE2 GLU A 135  -19.775  47.640 -13.732  1.00 53.57  A O
ATOM   781  C   GLU A 135  -15.650  48.768 -16.193  1.00 53.27  A C
ATOM   782  O   GLU A 135  -15.912  49.337 -17.254  1.00 54.08  A O
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FIGURE 1A-15

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ATOM  783  N   ARG A 136  -14.923  49.336 -15.234  1.00 51.80  A N
ATOM  784  CA  ARG A 136  -14.398  50.686 -15.402  1.00 51.30  A C
ATOM  785  CB  ARG A 136  -14.433  51.450 -14.089  1.00 53.99  A C
ATOM  786  CG  ARG A 136  -15.781  51.684 -13.457  1.00 56.96  A C
ATOM  787  CD  ARG A 136  -15.568  52.787 -12.441  1.00 59.02  A C
ATOM  788  NE  ARG A 136  -16.735  53.076 -11.628  1.00 60.30  A N
ATOM  789  CZ  ARG A 136  -16.844  54.159 -10.866  1.00 60.06  A C
ATOM  790  NH1 ARG A 136  -15.852  55.046 -10.827  1.00 57.80  A N
ATOM  791  NH2 ARG A 136  -17.942  54.352 -10.143  1.00 60.23  A N
ATOM  792  C   ARG A 136  -12.969  50.753 -15.904  1.00 49.84  A C
ATOM  793  O   ARG A 136  -12.485  51.831 -16.231  1.00 50.31  A O
ATOM  794  N   GLY A 137  -12.281  49.619 -15.940  1.00 48.73  A N
ATOM  795  CA  GLY A 137  -10.896  49.632 -16.382  1.00 46.25  A C
ATOM  796  C   GLY A 137   -9.995  50.228 -15.308  1.00 43.89  A C
ATOM  797  O   GLY A 137  -10.391  50.327 -14.145  1.00 42.31  A O
ATOM  798  N   ALA A 138   -8.787  50.630 -15.696  1.00 41.58  A N
ATOM  799  CA  ALA A 138   -7.829  51.214 -14.765  1.00 39.50  A C
ATOM  800  CB  ALA A 138   -6.631  51.745 -15.526  1.00 38.37  A C
ATOM  801  C   ALA A 138   -8.468  52.328 -13.944  1.00 39.08  A C
ATOM  802  O   ALA A 138   -9.287  53.100 -14.454  1.00 40.34  A O
ATOM  803  N   LEU A 139   -8.085  52.414 -12.674  1.00 37.49  A N
ATOM  804  CA  LEU A 139   -8.630  53.418 -11.771  1.00 36.03  A C
ATOM  805  CB  LEU A 139   -8.804  52.828 -10.371  1.00 33.89  A C
ATOM  806  CG  LEU A 139   -9.534  51.493 -10.230  1.00 35.16  A C
ATOM  807  CD1 LEU A 139   -9.629  51.130  -8.745  1.00 32.91  A C
ATOM  808  CD2 LEU A 139  -10.928  51.595 -10.848  1.00 33.06  A C
ATOM  809  C   LEU A 139   -7.743  54.647 -11.660  1.00 36.58  A C
ATOM  810  O   LEU A 139   -6.513  54.547 -11.730  1.00 36.36  A O
ATOM  811  N   GLN A 140   -8.374  55.807 -11.489  1.00 34.62  A N
ATOM  812  CA  GLN A 140   -7.638  57.050 -11.316  1.00 36.04  A C
ATOM  813  CB  GLN A 140   -8.592  58.238 -11.245  1.00 37.52  A C
ATOM  814  CG  GLN A 140   -9.425  58.420 -12.506  1.00 44.14  A C
ATOM  815  CD  GLN A 140  -10.424  59.566 -12.399  1.00 47.38  A C
ATOM  816  OE1 GLN A 140  -11.261  59.752 -13.286  1.00 49.91  A O
ATOM  817  NE2 GLN A 140  -10.338  60.341 -11.312  1.00 45.77  A N
ATOM  818  C   GLN A 140   -6.914  56.872  -9.990  1.00 35.45  A C
ATOM  819  O   GLN A 140   -7.433  56.221  -9.086  1.00 35.46  A O
ATOM  820  N   GLU A 141   -5.728  57.454  -9.870  1.00 34.91  A N
ATOM  821  CA  GLU A 141   -4.928  57.292  -8.663  1.00 35.54  A C
ATOM  822  CB  GLU A 141   -3.559  57.945  -8.872  1.00 33.61  A C
ATOM  823  CG  GLU A 141   -2.849  57.317 -10.075  1.00 34.48  A C
ATOM  824  CD  GLU A 141   -1.377  57.649 -10.172  1.00 34.92  A C
ATOM  825  OE1 GLU A 141   -0.767  57.307 -11.206  1.00 37.90  A O
ATOM  826  OE2 GLU A 141   -0.822  58.241  -9.227  1.00 34.50  A O
ATOM  827  C   GLU A 141   -5.561  57.731  -7.354  1.00 35.34  A C
ATOM  828  O   GLU A 141   -5.286  57.155  -6.304  1.00 37.17  A O
ATOM  829  N   GLU A 142   -6.422  58.734  -7.411  1.00 35.69  A N
ATOM  830  CA  GLU A 142   -7.096  59.208  -6.213  1.00 34.86  A C
ATOM  831  CB  GLU A 142   -7.918  60.453  -6.549  1.00 36.40  A C
ATOM  832  CG  GLU A 142   -8.914  60.859  -5.490  1.00 41.18  A C
ATOM  833  CD  GLU A 142   -9.624  62.156  -5.840  1.00 43.46  A C
ATOM  834  OE1 GLU A 142   -9.035  63.237  -5.607  1.00 45.28  A O
ATOM  835  OE2 GLU A 142  -10.763  62.089  -6.356  1.00 43.37  A O
ATOM  836  C   GLU A 142   -8.005  58.096  -5.688  1.00 32.39  A C
ATOM  837  O   GLU A 142   -8.090  57.856  -4.490  1.00 32.11  A O
ATOM  838  N   LEU A 143   -8.679  57.410  -6.594  1.00 31.13  A N
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FIGURE 1A-16

```
ATOM  839  CA  LEU A 143    -9.571  56.329  -6.202  1.00 31.68  A C
ATOM  840  CB  LEU A 143   -10.453  55.947  -7.390  1.00 30.38  A C
ATOM  841  CG  LEU A 143   -11.520  54.878  -7.213  1.00 31.57  A C
ATOM  842  CD1 LEU A 143   -12.446  55.239  -6.066  1.00 32.39  A C
ATOM  843  CD2 LEU A 143   -12.284  54.740  -8.518  1.00 30.05  A C
ATOM  844  C   LEU A 143    -8.737  55.133  -5.736  1.00 30.95  A C
ATOM  845  O   LEU A 143    -9.025  54.521  -4.708  1.00 31.34  A O
ATOM  846  N   ALA A 144    -7.690  54.813  -6.486  1.00 29.35  A N
ATOM  847  CA  ALA A 144    -6.825  53.695  -6.126  1.00 29.38  A C
ATOM  848  CB  ALA A 144    -5.758  53.495  -7.185  1.00 26.00  A C
ATOM  849  C   ALA A 144    -6.179  53.956  -4.767  1.00 29.15  A C
ATOM  850  O   ALA A 144    -5.957  53.025  -3.993  1.00 28.70  A O
ATOM  851  N   ARG A 145    -5.906  55.229  -4.476  1.00 29.20  A N
ATOM  852  CA  ARG A 145    -5.277  55.608  -3.214  1.00 30.72  A C
ATOM  853  CB  ARG A 145    -4.936  57.102  -3.195  1.00 31.95  A C
ATOM  854  CG  ARG A 145    -3.742  57.429  -2.299  1.00 35.79  A C
ATOM  855  CD  ARG A 145    -3.500  58.932  -2.066  1.00 35.64  A C
ATOM  856  NE  ARG A 145    -4.037  59.814  -3.098  1.00 41.74  A N
ATOM  857  CZ  ARG A 145    -3.447  60.123  -4.250  1.00 42.74  A C
ATOM  858  NH1 ARG A 145    -2.263  59.625  -4.576  1.00 42.23  A N
ATOM  859  NH2 ARG A 145    -4.045  60.970  -5.072  1.00 45.88  A N
ATOM  860  C   ARG A 145    -6.205  55.309  -2.051  1.00 30.15  A C
ATOM  861  O   ARG A 145    -5.797  54.723  -1.046  1.00 30.68  A O
ATOM  862  N   SER A 146    -7.456  55.723  -2.192  1.00 29.59  A N
ATOM  863  CA  SER A 146    -8.451  55.512  -1.148  1.00 30.04  A C
ATOM  864  CB  SER A 146    -9.757  56.214  -1.535  1.00 29.80  A C
ATOM  865  OG  SER A 146   -10.822  55.813  -0.695  1.00 32.64  A O
ATOM  866  C   SER A 146    -8.689  54.020  -0.932  1.00 29.85  A C
ATOM  867  O   SER A 146    -8.732  53.545   0.206  1.00 28.62  A O
ATOM  868  N   PHE A 147    -8.834  53.287  -2.035  1.00 29.40  A N
ATOM  869  CA  PHE A 147    -9.057  51.849  -1.972  1.00 29.31  A C
ATOM  870  CB  PHE A 147    -9.305  51.281  -3.382  1.00 30.27  A C
ATOM  871  CG  PHE A 147   -10.703  51.532  -3.909  1.00 32.52  A C
ATOM  872  CD1 PHE A 147   -11.125  50.953  -5.104  1.00 30.99  A C
ATOM  873  CD2 PHE A 147   -11.610  52.325  -3.196  1.00 30.39  A C
ATOM  874  CE1 PHE A 147   -12.424  51.154  -5.581  1.00 29.58  A C
ATOM  875  CE2 PHE A 147   -12.905  52.530  -3.667  1.00 31.05  A C
ATOM  876  CZ  PHE A 147   -13.311  51.941  -4.861  1.00 31.71  A C
ATOM  877  C   PHE A 147    -7.879  51.118  -1.326  1.00 29.36  A C
ATOM  878  O   PHE A 147    -8.058  50.331  -0.393  1.00 28.72  A O
ATOM  879  N   PHE A 148    -6.676  51.390  -1.823  1.00 27.89  A N
ATOM  880  CA  PHE A 148    -5.474  50.748  -1.314  1.00 28.44  A C
ATOM  881  CB  PHE A 148    -4.248  51.240  -2.098  1.00 27.56  A C
ATOM  882  CG  PHE A 148    -3.018  50.398  -1.895  1.00 29.31  A C
ATOM  883  CD1 PHE A 148    -3.003  49.061  -2.284  1.00 28.64  A C
ATOM  884  CD2 PHE A 148    -1.872  50.939  -1.317  1.00 29.34  A C
ATOM  885  CE1 PHE A 148    -1.863  48.269  -2.102  1.00 28.55  A C
ATOM  886  CE2 PHE A 148    -0.725  50.154  -1.131  1.00 28.09  A C
ATOM  887  CZ  PHE A 148    -0.722  48.819  -1.525  1.00 26.51  A C
ATOM  888  C   PHE A 148    -5.319  51.065   0.175  1.00 27.72  A C
ATOM  889  O   PHE A 148    -5.057  50.172   0.991  1.00 27.58  A O
ATOM  890  N   TRP A 149    -5.489  52.337   0.525  1.00 26.46  A N
ATOM  891  CA  TRP A 149    -5.377  52.758   1.916  1.00 27.15  A C
ATOM  892  CB  TRP A 149    -5.735  54.244   2.054  1.00 27.07  A C
ATOM  893  CG  TRP A 149    -5.566  54.776   3.440  1.00 27.44  A C
ATOM  894  CD2 TRP A 149    -4.356  55.282   4.027  1.00 28.29  A C
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FIGURE 1A-17

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ATOM  895  CE2 TRP A 149    -4.652  55.622   5.358  1.00 27.87   A C
ATOM  896  CE3 TRP A 149    -3.050  55.476   3.554  1.00 29.66   A C
ATOM  897  CD1 TRP A 149    -6.511  54.832   4.408  1.00 27.87   A C
ATOM  898  NE1 TRP A 149    -5.974  55.337   5.566  1.00 27.58   A N
ATOM  899  CZ2 TRP A 149    -3.692  56.153   6.230  1.00 30.01   A C
ATOM  900  CZ3 TRP A 149    -2.094  56.001   4.418  1.00 31.11   A C
ATOM  901  CH2 TRP A 149    -2.422  56.332   5.743  1.00 30.52   A C
ATOM  902  C   TRP A 149    -6.292  51.904   2.800  1.00 27.70   A C
ATOM  903  O   TRP A 149    -5.843  51.360   3.814  1.00 26.51   A O
ATOM  904  N   GLN A 150    -7.559  51.758   2.405  1.00 26.97   A N
ATOM  905  CA  GLN A 150    -8.499  50.967   3.197  1.00 27.64   A C
ATOM  906  CB  GLN A 150    -9.924  51.087   2.639  1.00 27.64   A C
ATOM  907  CG  GLN A 150   -10.531  52.477   2.781  1.00 29.11   A C
ATOM  908  CD  GLN A 150   -11.975  52.528   2.325  1.00 32.37   A C
ATOM  909  OE1 GLN A 150   -12.803  51.711   2.738  1.00 33.04   A O
ATOM  910  NE2 GLN A 150   -12.286  53.491   1.474  1.00 32.60   A N
ATOM  911  C   GLN A 150    -8.097  49.497   3.274  1.00 28.91   A C
ATOM  912  O   GLN A 150    -8.328  48.836   4.292  1.00 28.31   A O
ATOM  913  N   VAL A 151    -7.516  48.970   2.200  1.00 28.46   A N
ATOM  914  CA  VAL A 151    -7.085  47.582   2.232  1.00 30.71   A C
ATOM  915  CB  VAL A 151    -6.577  47.108   0.865  1.00 31.71   A C
ATOM  916  CG1 VAL A 151    -5.932  45.744   1.005  1.00 31.67   A C
ATOM  917  CG2 VAL A 151    -7.749  47.028  -0.119  1.00 33.89   A C
ATOM  918  C   VAL A 151    -5.961  47.461   3.255  1.00 30.47   A C
ATOM  919  O   VAL A 151    -5.901  46.498   4.015  1.00 29.97   A O
ATOM  920  N   LEU A 152    -5.080  48.454   3.287  1.00 30.38   A N
ATOM  921  CA  LEU A 152    -3.977  48.437   4.238  1.00 31.04   A C
ATOM  922  CB  LEU A 152    -3.024  49.594   3.950  1.00 31.42   A C
ATOM  923  CG  LEU A 152    -1.962  49.218   2.915  1.00 33.37   A C
ATOM  924  CD1 LEU A 152    -1.637  50.418   2.083  1.00 34.79   A C
ATOM  925  CD2 LEU A 152    -0.709  48.673   3.627  1.00 31.32   A C
ATOM  926  C   LEU A 152    -4.448  48.496   5.688  1.00 31.47   A C
ATOM  927  O   LEU A 152    -3.875  47.825   6.560  1.00 32.88   A O
ATOM  928  N   GLU A 153    -5.475  49.300   5.958  1.00 28.51   A N
ATOM  929  CA  GLU A 153    -5.993  49.398   7.316  1.00 28.60   A C
ATOM  930  CB  GLU A 153    -7.065  50.487   7.424  1.00 28.63   A C
ATOM  931  CG  GLU A 153    -6.528  51.906   7.363  1.00 30.20   A C
ATOM  932  CD  GLU A 153    -5.752  52.304   8.609  1.00 30.76   A C
ATOM  933  OE1 GLU A 153    -4.654  52.862   8.447  1.00 31.11   A O
ATOM  934  OE2 GLU A 153    -6.238  52.078   9.741  1.00 31.44   A O
ATOM  935  C   GLU A 153    -6.606  48.066   7.709  1.00 27.63   A C
ATOM  936  O   GLU A 153    -6.524  47.648   8.862  1.00 27.01   A O
ATOM  937  N   ALA A 154    -7.214  47.394   6.739  1.00 27.72   A N
ATOM  938  CA  ALA A 154    -7.865  46.113   6.994  1.00 28.64   A C
ATOM  939  CB  ALA A 154    -8.772  45.740   5.814  1.00 25.00   A C
ATOM  940  C   ALA A 154    -6.849  45.011   7.241  1.00 29.79   A C
ATOM  941  O   ALA A 154    -7.039  44.146   8.099  1.00 29.36   A O
ATOM  942  N   VAL A 155    -5.763  45.042   6.480  1.00 31.28   A N
ATOM  943  CA  VAL A 155    -4.732  44.035   6.630  1.00 31.67   A C
ATOM  944  CB  VAL A 155    -3.736  44.104   5.468  1.00 31.42   A C
ATOM  945  CG1 VAL A 155    -2.624  43.120   5.676  1.00 35.39   A C
ATOM  946  CG2 VAL A 155    -4.461  43.763   4.176  1.00 31.51   A C
ATOM  947  C   VAL A 155    -4.048  44.239   7.970  1.00 32.30   A C
ATOM  948  O   VAL A 155    -3.751  43.267   8.668  1.00 33.13   A O
ATOM  949  N   ARG A 156    -3.824  45.496   8.346  1.00 30.46   A N
ATOM  950  CA  ARG A 156    -3.205  45.780   9.637  1.00 30.53   A C
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FIGURE 1A-18

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ATOM   951  CB  ARG A 156    -3.004  47.283   9.850  1.00 28.53   A C
ATOM   952  CG  ARG A 156    -1.916  47.897   8.982  1.00 29.04   A C
ATOM   953  CD  ARG A 156    -1.830  49.389   9.230  1.00 28.05   A C
ATOM   954  NE  ARG A 156    -1.597  49.683  10.640  1.00 27.71   A N
ATOM   955  CZ  ARG A 156    -1.737  50.886  11.189  1.00 28.51   A C
ATOM   956 NH1  ARG A 156    -2.116  51.927  10.451  1.00 27.84   A N
ATOM   957 NH2  ARG A 156    -1.496  51.049  12.482  1.00 28.52   A N
ATOM   958  C   ARG A 156    -4.117  45.244  10.722  1.00 31.26   A C
ATOM   959  O   ARG A 156    -3.652  44.678  11.703  1.00 31.87   A O
ATOM   960  N   HIS A 157    -5.422  45.428  10.533  1.00 32.57   A N
ATOM   961  CA  HIS A 157    -6.416  44.954  11.488  1.00 34.30   A C
ATOM   962  CB  HIS A 157    -7.830  45.244  10.974  1.00 34.75   A C
ATOM   963  CG  HIS A 157    -8.908  44.562  11.758  1.00 38.53   A C
ATOM   964 CD2  HIS A 157    -9.812  43.615  11.397  1.00 38.29   A C
ATOM   965 ND1  HIS A 157    -9.142  44.823  13.093  1.00 40.22   A N
ATOM   966 CE1  HIS A 157   -10.141  44.068  13.520  1.00 38.11   A C
ATOM   967 NE2  HIS A 157   -10.564  43.328  12.510  1.00 39.40   A N
ATOM   968  C   HIS A 157    -6.255  43.457  11.712  1.00 34.05   A C
ATOM   969  O   HIS A 157    -6.095  43.023  12.839  1.00 34.54   A O
ATOM   970  N   CYS A 158    -6.287  42.676  10.632  1.00 33.34   A N
ATOM   971  CA  CYS A 158    -6.140  41.221  10.726  1.00 32.06   A C
ATOM   972  CB  CYS A 158    -6.160  40.586   9.337  1.00 31.07   A C
ATOM   973  SG  CYS A 158    -7.675  40.824   8.422  1.00 34.98   A S
ATOM   974  C   CYS A 158    -4.845  40.813  11.415  1.00 32.56   A C
ATOM   975  O   CYS A 158    -4.848  39.958  12.301  1.00 31.24   A O
ATOM   976  N   HIS A 159    -3.733  41.412  10.989  1.00 33.90   A N
ATOM   977  CA  HIS A 159    -2.425  41.101  11.566  1.00 35.83   A C
ATOM   978  CB  HIS A 159    -1.333  41.909  10.866  1.00 37.68   A C
ATOM   979  CG  HIS A 159    -1.022  41.423   9.482  1.00 42.89   A C
ATOM   980 CD2  HIS A 159     0.119  41.472   8.754  1.00 44.16   A C
ATOM   981 ND1  HIS A 159    -1.962  40.815   8.675  1.00 46.47   A N
ATOM   982 CE1  HIS A 159    -1.415  40.513   7.511  1.00 45.44   A C
ATOM   983 NE2  HIS A 159    -0.153  40.902   7.532  1.00 45.62   A N
ATOM   984  C   HIS A 159    -2.435  41.388  13.056  1.00 36.31   A C
ATOM   985  O   HIS A 159    -2.009  40.568  13.860  1.00 35.42   A O
ATOM   986  N   ASN A 160    -2.950  42.550  13.418  1.00 38.20   A N
ATOM   987  CA  ASN A 160    -3.041  42.942  14.810  1.00 40.64   A C
ATOM   988  CB  ASN A 160    -3.672  44.326  14.893  1.00 44.28   A C
ATOM   989  CG  ASN A 160    -3.608  44.911  16.278  1.00 50.19   A C
ATOM   990 OD1  ASN A 160    -4.317  44.473  17.191  1.00 53.38   A O
ATOM   991 ND2  ASN A 160    -2.748  45.912  16.451  1.00 53.81   A N
ATOM   992  C   ASN A 160    -3.881  41.918  15.590  1.00 41.56   A C
ATOM   993  O   ASN A 160    -3.693  41.729  16.791  1.00 39.72   A O
ATOM   994  N   CME A 161    -4.797  41.248  14.894  1.00 41.66   A N
ATOM   995  CA  CME A 161    -5.658  40.256  15.523  1.00 41.26   A C
ATOM   996  C   CME A 161    -5.074  38.849  15.441  1.00 39.56   A C
ATOM   997  CB  CME A 161    -7.045  40.269  14.874  1.00 44.58   A C
ATOM   998  SG  CME A 161    -8.106  41.675  15.306  1.00 48.71   A S
ATOM   999  S1  CME A 161    -8.208  41.714  17.450  1.00 63.10   A S
ATOM  1000  C1  CME A 161    -7.508  43.318  17.982  1.00 61.90   A C
ATOM  1001  C2  CME A 161    -8.594  44.086  18.735  1.00 66.41   A C
ATOM  1002  O1  CME A 161    -8.606  45.481  18.378  1.00 67.54   A O
ATOM  1003  O   CME A 161    -5.719  37.890  15.853  1.00 38.26   A O
ATOM  1004  N   GLY A 162    -3.861  38.735  14.900  1.00 37.87   A N
ATOM  1005  CA  GLY A 162    -3.201  37.444  14.782  1.00 35.74   A C
ATOM  1006  C   GLY A 162    -3.587  36.637  13.554  1.00 36.04   A C
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FIGURE 1A-19

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ATOM 1007  O   GLY A 162   -3.298  35.438  13.466  1.00 36.09  A O
ATOM 1008  N   VAL A 163   -4.230  37.292  12.593  1.00 34.77  A N
ATOM 1009  CA  VAL A 163   -4.662  36.616  11.381  1.00 33.02  A C
ATOM 1010  CB  VAL A 163   -6.163  36.777  11.197  1.00 33.05  A C
ATOM 1011  CG1 VAL A 163   -6.601  36.125   9.899  1.00 32.86  A C
ATOM 1012  CG2 VAL A 163   -6.888  36.174  12.388  1.00 33.86  A C
ATOM 1013  C   VAL A 163   -3.974  37.085  10.099  1.00 34.02  A C
ATOM 1014  O   VAL A 163   -3.790  38.281   9.869  1.00 33.49  A O
ATOM 1015  N   LEU A 164   -3.611  36.126   9.257  1.00 34.37  A N
ATOM 1016  CA  LEU A 164   -2.964  36.418   7.981  1.00 34.89  A C
ATOM 1017  CB  LEU A 164   -1.640  35.666   7.920  1.00 35.78  A C
ATOM 1018  CG  LEU A 164   -0.616  36.048   6.860  1.00 37.54  A C
ATOM 1019  CD1 LEU A 164   -0.115  37.462   7.119  1.00 37.00  A C
ATOM 1020  CD2 LEU A 164    0.536  35.049   6.907  1.00 39.22  A C
ATOM 1021  C   LEU A 164   -3.924  35.916   6.894  1.00 34.36  A C
ATOM 1022  O   LEU A 164   -4.237  34.722   6.841  1.00 36.04  A O
ATOM 1023  N   HIS A 165   -4.407  36.808   6.036  1.00 33.55  A N
ATOM 1024  CA  HIS A 165   -5.358  36.399   4.996  1.00 31.81  A C
ATOM 1025  CB  HIS A 165   -5.948  37.641   4.323  1.00 31.48  A C
ATOM 1026  CG  HIS A 165   -7.061  37.353   3.359  1.00 30.10  A C
ATOM 1027  CD2 HIS A 165   -8.387  37.612   3.429  1.00 29.57  A C
ATOM 1028  ND1 HIS A 165   -6.852  36.764   2.130  1.00 28.84  A N
ATOM 1029  CE1 HIS A 165   -8.000  36.676   1.485  1.00 29.55  A C
ATOM 1030  NE2 HIS A 165   -8.947  37.184   2.250  1.00 28.68  A N
ATOM 1031  C   HIS A 165   -4.768  35.450   3.948  1.00 33.67  A C
ATOM 1032  O   HIS A 165   -5.389  34.444   3.598  1.00 34.16  A O
ATOM 1033  N   ARG A 166   -3.580  35.769   3.442  1.00 33.74  A N
ATOM 1034  CA  ARG A 166   -2.901  34.929   2.449  1.00 34.00  A C
ATOM 1035  CB  ARG A 166   -2.796  33.496   2.947  1.00 34.85  A C
ATOM 1036  CG  ARG A 166   -2.045  33.357   4.242  1.00 38.62  A C
ATOM 1037  CD  ARG A 166   -2.360  32.015   4.849  1.00 42.19  A C
ATOM 1038  NE  ARG A 166   -1.266  31.073   4.695  1.00 42.06  A N
ATOM 1039  CZ  ARG A 166   -1.398  29.762   4.859  1.00 43.51  A C
ATOM 1040  NH1 ARG A 166   -2.585  29.246   5.172  1.00 40.24  A N
ATOM 1041  NH2 ARG A 166   -0.338  28.971   4.730  1.00 43.30  A N
ATOM 1042  C   ARG A 166   -3.496  34.894   1.051  1.00 34.98  A C
ATOM 1043  O   ARG A 166   -2.962  34.210   0.181  1.00 36.36  A O
ATOM 1044  N   ASP A 167   -4.591  35.602   0.816  1.00 34.53  A N
ATOM 1045  CA  ASP A 167   -5.162  35.598  -0.521  1.00 36.40  A C
ATOM 1046  CB  ASP A 167   -6.208  34.486  -0.632  1.00 39.34  A C
ATOM 1047  CG  ASP A 167   -6.544  34.133  -2.076  1.00 41.91  A C
ATOM 1048  OD1 ASP A 167   -5.651  34.235  -2.947  1.00 42.15  A O
ATOM 1049  OD2 ASP A 167   -7.704  33.735  -2.331  1.00 44.45  A O
ATOM 1050  C   ASP A 167   -5.767  36.956  -0.878  1.00 36.51  A C
ATOM 1051  O   ASP A 167   -6.870  37.042  -1.418  1.00 35.57  A O
ATOM 1052  N   ILE A 168   -5.026  38.018  -0.569  1.00 36.07  A N
ATOM 1053  CA  ILE A 168   -5.468  39.371  -0.861  1.00 35.99  A C
ATOM 1054  CB  ILE A 168   -4.530  40.405  -0.199  1.00 38.45  A C
ATOM 1055  CG2 ILE A 168   -4.923  41.820  -0.613  1.00 37.35  A C
ATOM 1056  CG1 ILE A 168   -4.576  40.259   1.323  1.00 37.67  A C
ATOM 1057  CD1 ILE A 168   -3.450  40.983   2.021  1.00 37.95  A C
ATOM 1058  C   ILE A 168   -5.428  39.556  -2.377  1.00 36.21  A C
ATOM 1059  O   ILE A 168   -4.399  39.318  -3.005  1.00 36.83  A O
ATOM 1060  N   LYS A 169   -6.554  39.963  -2.958  1.00 35.75  A N
ATOM 1061  CA  LYS A 169   -6.666  40.193  -4.399  1.00 36.29  A C
ATOM 1062  CB  LYS A 169   -6.523  38.880  -5.184  1.00 37.33  A C
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FIGURE 1A-20

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ATOM 1063  CG  LYS A 169    -7.656  37.898  -4.973  1.00 40.26  A C
ATOM 1064  CD  LYS A 169    -7.490  36.635  -5.800  1.00 42.71  A C
ATOM 1065  CE  LYS A 169    -8.612  35.657  -5.469  1.00 45.20  A C
ATOM 1066  NZ  LYS A 169    -8.528  34.383  -6.238  1.00 49.93  A N
ATOM 1067  C   LYS A 169    -8.023  40.838  -4.699  1.00 36.42  A C
ATOM 1068  O   LYS A 169    -8.918  40.839  -3.844  1.00 34.37  A O
ATOM 1069  N   ASP A 170    -8.180  41.373  -5.909  1.00 35.91  A N
ATOM 1070  CA  ASP A 170    -9.416  42.057  -6.279  1.00 37.63  A C
ATOM 1071  CB  ASP A 170    -9.405  42.444  -7.771  1.00 36.26  A C
ATOM 1072  CG  ASP A 170    -9.007  41.296  -8.683  1.00 35.59  A C
ATOM 1073  OD1 ASP A 170    -8.982  40.132  -8.240  1.00 37.22  A O
ATOM 1074  OD2 ASP A 170    -8.716  41.565  -9.862  1.00 38.04  A O
ATOM 1075  C   ASP A 170   -10.697  41.300  -5.945  1.00 38.50  A C
ATOM 1076  O   ASP A 170   -11.616  41.869  -5.354  1.00 39.90  A O
ATOM 1077  N   GLU A 171   -10.750  40.026  -6.313  1.00 38.22  A N
ATOM 1078  CA  GLU A 171   -11.917  39.182  -6.060  1.00 40.07  A C
ATOM 1079  CB  GLU A 171   -11.690  37.779  -6.629  1.00 43.50  A C
ATOM 1080  CG  GLU A 171   -11.531  37.746  -8.138  1.00 51.40  A C
ATOM 1081  CD  GLU A 171   -11.067  36.392  -8.657  1.00 55.72  A C
ATOM 1082  OE1 GLU A 171    -9.898  36.019  -8.403  1.00 58.56  A O
ATOM 1083  OE2 GLU A 171   -11.875  35.701  -9.318  1.00 58.36  A O
ATOM 1084  C   GLU A 171   -12.288  39.050  -4.592  1.00 37.88  A C
ATOM 1085  O   GLU A 171   -13.444  38.798  -4.272  1.00 39.07  A O
ATOM 1086  N   ASN A 172   -11.316  39.210  -3.700  1.00 36.72  A N
ATOM 1087  CA  ASN A 172   -11.591  39.080  -2.277  1.00 34.84  A C
ATOM 1088  CB  ASN A 172   -10.493  38.255  -1.597  1.00 33.95  A C
ATOM 1089  CG  ASN A 172   -10.536  36.791  -2.014  1.00 35.75  A C
ATOM 1090  OD1 ASN A 172   -11.614  36.255  -2.281  1.00 36.01  A O
ATOM 1091  ND2 ASN A 172    -9.377  36.135  -2.061  1.00 32.53  A N
ATOM 1092  C   ASN A 172   -11.790  40.406  -1.570  1.00 34.79  A C
ATOM 1093  O   ASN A 172   -11.710  40.492  -0.337  1.00 36.01  A O
ATOM 1094  N   ILE A 173   -12.064  41.438  -2.362  1.00 34.41  A N
ATOM 1095  CA  ILE A 173   -12.311  42.776  -1.842  1.00 33.58  A C
ATOM 1096  CB  ILE A 173   -11.247  43.762  -2.347  1.00 34.06  A C
ATOM 1097  CG2 ILE A 173   -11.564  45.171  -1.863  1.00 31.76  A C
ATOM 1098  CG1 ILE A 173    -9.862  43.310  -1.874  1.00 33.08  A C
ATOM 1099  CD1 ILE A 173    -8.731  44.155  -2.396  1.00 31.22  A C
ATOM 1100  C   ILE A 173   -13.704  43.240  -2.309  1.00 34.69  A C
ATOM 1101  O   ILE A 173   -13.979  43.309  -3.510  1.00 33.81  A O
ATOM 1102  N   LEU A 174   -14.578  43.534  -1.351  1.00 34.57  A N
ATOM 1103  CA  LEU A 174   -15.936  43.988  -1.636  1.00 36.37  A C
ATOM 1104  CB  LEU A 174   -16.935  43.335  -0.688  1.00 36.56  A C
ATOM 1105  CG  LEU A 174   -17.777  42.185  -1.213  1.00 37.78  A C
ATOM 1106  CD1 LEU A 174   -16.896  41.140  -1.863  1.00 38.44  A C
ATOM 1107  CD2 LEU A 174   -18.572  41.604  -0.052  1.00 38.08  A C
ATOM 1108  C   LEU A 174   -16.045  45.480  -1.457  1.00 37.08  A C
ATOM 1109  O   LEU A 174   -15.502  46.036  -0.495  1.00 36.65  A O
ATOM 1110  N   ILE A 175   -16.757  46.128  -2.373  1.00 36.94  A N
ATOM 1111  CA  ILE A 175   -16.947  47.567  -2.285  1.00 38.73  A C
ATOM 1112  CB  ILE A 175   -16.634  48.273  -3.616  1.00 38.83  A C
ATOM 1113  CG2 ILE A 175   -16.609  49.781  -3.401  1.00 37.29  A C
ATOM 1114  CG1 ILE A 175   -15.289  47.813  -4.163  1.00 38.35  A C
ATOM 1115  CD1 ILE A 175   -15.064  48.237  -5.587  1.00 39.97  A C
ATOM 1116  C   ILE A 175   -18.392  47.910  -1.926  1.00 40.86  A C
ATOM 1117  O   ILE A 175   -19.340  47.491  -2.599  1.00 42.27  A O
ATOM 1118  N   ASP A 176   -18.563  48.662  -0.852  1.00 41.41  A N
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FIGURE 1A-21

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ATOM 1119  CA  ASP A 176  -19.887  49.105  -0.446  1.00 42.09  A C
ATOM 1120  CB  ASP A 176  -19.898  49.305   1.071  1.00 42.04  A C
ATOM 1121  CG  ASP A 176  -21.154  49.967   1.570  1.00 44.89  A C
ATOM 1122  OD1 ASP A 176  -21.450  49.810   2.778  1.00 43.98  A O
ATOM 1123  OD2 ASP A 176  -21.829  50.656   0.770  1.00 45.38  A O
ATOM 1124  C   ASP A 176  -20.051  50.427  -1.205  1.00 42.45  A C
ATOM 1125  O   ASP A 176  -19.579  51.470  -0.752  1.00 41.94  A O
ATOM 1126  N   LEU A 177  -20.696  50.368  -2.372  1.00 42.39  A N
ATOM 1127  CA  LEU A 177  -20.885  51.548  -3.222  1.00 43.16  A C
ATOM 1128  CB  LEU A 177  -21.768  51.220  -4.431  1.00 41.21  A C
ATOM 1129  CG  LEU A 177  -21.314  50.291  -5.565  1.00 40.68  A C
ATOM 1130  CD1 LEU A 177  -19.788  50.316  -5.718  1.00 35.16  A C
ATOM 1131  CD2 LEU A 177  -21.814  48.895  -5.282  1.00 39.32  A C
ATOM 1132  C   LEU A 177  -21.426  52.834  -2.594  1.00 45.22  A C
ATOM 1133  O   LEU A 177  -21.061  53.926  -3.028  1.00 46.52  A O
ATOM 1134  N   ASN A 178  -22.290  52.728  -1.591  1.00 45.69  A N
ATOM 1135  CA  ASN A 178  -22.849  53.931  -0.975  1.00 46.91  A C
ATOM 1136  CB  ASN A 178  -24.241  53.633  -0.413  1.00 48.88  A C
ATOM 1137  CG  ASN A 178  -25.291  53.457  -1.505  1.00 51.18  A C
ATOM 1138  OD1 ASN A 178  -26.437  53.104  -1.226  1.00 53.57  A O
ATOM 1139  ND2 ASN A 178  -24.904  53.708  -2.754  1.00 52.84  A N
ATOM 1140  C   ASN A 178  -21.989  54.594   0.107  1.00 47.21  A C
ATOM 1141  O   ASN A 178  -21.963  55.826   0.208  1.00 47.38  A O
ATOM 1142  N   ARG A 179  -21.290  53.800   0.916  1.00 46.57  A N
ATOM 1143  CA  ARG A 179  -20.452  54.382   1.967  1.00 46.14  A C
ATOM 1144  CB  ARG A 179  -20.489  53.522   3.234  1.00 47.75  A C
ATOM 1145  CG  ARG A 179  -21.808  52.805   3.451  1.00 51.15  A C
ATOM 1146  CD  ARG A 179  -22.088  52.548   4.921  1.00 53.20  A C
ATOM 1147  NE  ARG A 179  -22.544  53.766   5.581  1.00 57.25  A N
ATOM 1148  CZ  ARG A 179  -23.262  53.788   6.700  1.00 58.29  A C
ATOM 1149  NH1 ARG A 179  -23.606  52.648   7.289  1.00 59.75  A N
ATOM 1150  NH2 ARG A 179  -23.648  54.948   7.223  1.00 58.17  A N
ATOM 1151  C   ARG A 179  -19.006  54.545   1.506  1.00 44.47  A C
ATOM 1152  O   ARG A 179  -18.219  55.235   2.146  1.00 44.33  A O
ATOM 1153  N   GLY A 180  -18.666  53.914   0.387  1.00 42.12  A N
ATOM 1154  CA  GLY A 180  -17.310  54.009  -0.130  1.00 41.39  A C
ATOM 1155  C   GLY A 180  -16.284  53.218   0.672  1.00 39.63  A C
ATOM 1156  O   GLY A 180  -15.092  53.515   0.618  1.00 38.24  A O
ATOM 1157  N   GLU A 181  -16.746  52.206   1.401  1.00 37.87  A N
ATOM 1158  CA  GLU A 181  -15.867  51.380   2.219  1.00 37.67  A C
ATOM 1159  CB  GLU A 181  -16.477  51.186   3.606  1.00 36.35  A C
ATOM 1160  CG  GLU A 181  -17.341  52.340   4.058  1.00 39.49  A C
ATOM 1161  CD  GLU A 181  -17.762  52.223   5.505  1.00 40.40  A C
ATOM 1162  OE1 GLU A 181  -18.158  51.108   5.914  1.00 41.29  A O
ATOM 1163  OE2 GLU A 181  -17.702  53.248   6.224  1.00 39.82  A O
ATOM 1164  C   GLU A 181  -15.612  50.005   1.603  1.00 36.81  A C
ATOM 1165  O   GLU A 181  -16.522  49.394   1.043  1.00 36.23  A O
ATOM 1166  N   LEU A 182  -14.373  49.522   1.717  1.00 35.53  A N
ATOM 1167  CA  LEU A 182  -14.024  48.208   1.199  1.00 34.27  A C
ATOM 1168  CB  LEU A 182  -12.652  48.223   0.528  1.00 33.44  A C
ATOM 1169  CG  LEU A 182  -12.320  49.350  -0.446  1.00 36.60  A C
ATOM 1170  CD1 LEU A 182  -11.160  48.901  -1.333  1.00 35.63  A C
ATOM 1171  CD2 LEU A 182  -13.531  49.697  -1.298  1.00 36.56  A C
ATOM 1172  C   LEU A 182  -13.991  47.225   2.360  1.00 34.23  A C
ATOM 1173  O   LEU A 182  -13.700  47.607   3.497  1.00 32.59  A O
ATOM 1174  N   LYS A 183  -14.286  45.963   2.064  1.00 34.21  A N
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FIGURE 1A-22

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ATOM 1175  CA  LYS A 183  -14.279  44.908   3.071  1.00 36.94  A C
ATOM 1176  CB  LYS A 183  -15.712  44.609   3.526  1.00 39.85  A C
ATOM 1177  CG  LYS A 183  -16.364  45.770   4.239  1.00 43.30  A C
ATOM 1178  CD  LYS A 183  -17.748  45.415   4.743  1.00 46.84  A C
ATOM 1179  CE  LYS A 183  -18.381  46.621   5.415  1.00 49.08  A C
ATOM 1180  NZ  LYS A 183  -17.464  47.177   6.451  1.00 49.66  A N
ATOM 1181  C   LYS A 183  -13.622  43.629   2.544  1.00 36.53  A C
ATOM 1182  O   LYS A 183  -13.924  43.177   1.441  1.00 36.20  A O
ATOM 1183  N   LEU A 184  -12.723  43.050   3.335  1.00 36.01  A N
ATOM 1184  CA  LEU A 184  -12.032  41.823   2.944  1.00 36.20  A C
ATOM 1185  CB  LEU A 184  -10.796  41.615   3.810  1.00 36.61  A C
ATOM 1186  CG  LEU A 184   -9.444  42.046   3.249  1.00 40.20  A C
ATOM 1187  CD1 LEU A 184   -9.538  43.434   2.635  1.00 41.67  A C
ATOM 1188  CD2 LEU A 184   -8.424  42.023   4.374  1.00 40.75  A C
ATOM 1189  C   LEU A 184  -12.922  40.601   3.087  1.00 36.03  A C
ATOM 1190  O   LEU A 184  -13.683  40.502   4.048  1.00 34.41  A O
ATOM 1191  N   ILE A 185  -12.824  39.669   2.142  1.00 34.66  A N
ATOM 1192  CA  ILE A 185  -13.616  38.451   2.228  1.00 36.73  A C
ATOM 1193  CB  ILE A 185  -14.809  38.451   1.252  1.00 36.43  A C
ATOM 1194  CG2 ILE A 185  -15.750  39.605   1.575  1.00 38.39  A C
ATOM 1195  CG1 ILE A 185  -14.298  38.526  -0.184  1.00 36.83  A C
ATOM 1196  CD1 ILE A 185  -15.374  38.290  -1.220  1.00 36.70  A C
ATOM 1197  C   ILE A 185  -12.807  37.197   1.936  1.00 37.85  A C
ATOM 1198  O   ILE A 185  -11.715  37.259   1.358  1.00 37.03  A O
ATOM 1199  N   ASP A 186  -13.386  36.065   2.337  1.00 38.30  A N
ATOM 1200  CA  ASP A 186  -12.828  34.733   2.153  1.00 39.90  A C
ATOM 1201  CB  ASP A 186  -12.754  34.378   0.664  1.00 42.64  A C
ATOM 1202  CG  ASP A 186  -12.156  32.991   0.430  1.00 48.97  A C
ATOM 1203  OD1 ASP A 186  -12.648  32.024   1.061  1.00 48.12  A O
ATOM 1204  OD2 ASP A 186  -11.193  32.862  -0.372  1.00 53.28  A O
ATOM 1205  C   ASP A 186  -11.477  34.450   2.798  1.00 40.25  A C
ATOM 1206  O   ASP A 186  -10.435  34.494   2.141  1.00 39.75  A O
ATOM 1207  N   PHE A 187  -11.502  34.138   4.088  1.00 40.33  A N
ATOM 1208  CA  PHE A 187  -10.286  33.808   4.809  1.00 40.39  A C
ATOM 1209  CB  PHE A 187  -10.405  34.240   6.266  1.00 39.07  A C
ATOM 1210  CG  PHE A 187  -10.339  35.731   6.472  1.00 37.24  A C
ATOM 1211  CD1 PHE A 187  -11.394  36.549   6.094  1.00 35.91  A C
ATOM 1212  CD2 PHE A 187   -9.227  36.308   7.077  1.00 33.83  A C
ATOM 1213  CE1 PHE A 187  -11.344  37.920   6.319  1.00 35.51  A C
ATOM 1214  CE2 PHE A 187   -9.172  37.674   7.305  1.00 34.20  A C
ATOM 1215  CZ  PHE A 187  -10.227  38.481   6.929  1.00 34.86  A C
ATOM 1216  C   PHE A 187  -10.048  32.300   4.748  1.00 41.22  A C
ATOM 1217  O   PHE A 187   -9.362  31.738   5.597  1.00 42.04  A O
ATOM 1218  N   GLY A 188  -10.611  31.653   3.733  1.00 42.01  A N
ATOM 1219  CA  GLY A 188  -10.482  30.212   3.592  1.00 42.20  A C
ATOM 1220  C   GLY A 188   -9.097  29.688   3.289  1.00 43.07  A C
ATOM 1221  O   GLY A 188   -8.860  28.483   3.340  1.00 45.54  A O
ATOM 1222  N   SER A 189   -8.176  30.578   2.956  1.00 42.90  A N
ATOM 1223  CA  SER A 189   -6.809  30.166   2.662  1.00 42.57  A C
ATOM 1224  CB  SER A 189   -6.384  30.683   1.287  1.00 43.22  A C
ATOM 1225  OG  SER A 189   -7.227  30.191   0.259  1.00 46.25  A O
ATOM 1226  C   SER A 189   -5.907  30.769   3.724  1.00 41.36  A C
ATOM 1227  O   SER A 189   -4.695  30.638   3.668  1.00 41.93  A O
ATOM 1228  N   GLY A 190   -6.521  31.439   4.692  1.00 40.98  A N
ATOM 1229  CA  GLY A 190   -5.765  32.089   5.740  1.00 41.85  A C
ATOM 1230  C   GLY A 190   -5.037  31.171   6.696  1.00 42.01  A C
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FIGURE 1A-23

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ATOM 1231  O   GLY A 190   -5.044  29.952   6.548  1.00 41.06  A O
ATOM 1232  N   ALA A 191   -4.401  31.782   7.688  1.00 41.59  A N
ATOM 1233  CA  ALA A 191   -3.652  31.051   8.701  1.00 40.28  A C
ATOM 1234  CB  ALA A 191   -2.354  30.524   8.117  1.00 37.96  A C
ATOM 1235  C   ALA A 191   -3.357  32.002   9.838  1.00 39.49  A C
ATOM 1236  O   ALA A 191   -3.342  33.221   9.650  1.00 40.16  A O
ATOM 1237  N   LEU A 192   -3.143  31.450  11.023  1.00 39.39  A N
ATOM 1238  CA  LEU A 192   -2.823  32.265  12.181  1.00 38.58  A C
ATOM 1239  CB  LEU A 192   -2.691  31.379  13.420  1.00 37.99  A C
ATOM 1240  CG  LEU A 192   -3.965  30.645  13.850  1.00 38.01  A C
ATOM 1241  CD1 LEU A 192   -3.620  29.566  14.883  1.00 38.49  A C
ATOM 1242  CD2 LEU A 192   -4.964  31.648  14.423  1.00 35.85  A C
ATOM 1243  C   LEU A 192   -1.492  32.946  11.876  1.00 38.77  A C
ATOM 1244  O   LEU A 192   -0.611  32.356  11.241  1.00 38.52  A O
ATOM 1245  N   LEU A 193   -1.345  34.194  12.298  1.00 38.21  A N
ATOM 1246  CA  LEU A 193   -0.094  34.892  12.053  1.00 38.89  A C
ATOM 1247  CB  LEU A 193   -0.234  36.377  12.375  1.00 37.34  A C
ATOM 1248  CG  LEU A 193    1.036  37.197  12.100  1.00 37.45  A C
ATOM 1249  CD1 LEU A 193    1.298  37.230  10.590  1.00 34.06  A C
ATOM 1250  CD2 LEU A 193    0.874  38.626  12.654  1.00 35.69  A C
ATOM 1251  C   LEU A 193    1.008  34.302  12.929  1.00 39.70  A C
ATOM 1252  O   LEU A 193    0.806  34.079  14.124  1.00 39.90  A O
ATOM 1253  N   LYS A 194    2.164  34.037  12.330  1.00 39.29  A N
ATOM 1254  CA  LYS A 194    3.299  33.513  13.077  1.00 39.82  A C
ATOM 1255  CB  LYS A 194    3.381  31.981  12.971  1.00 39.34  A C
ATOM 1256  CG  LYS A 194    3.790  31.458  11.607  1.00 38.88  A C
ATOM 1257  CD  LYS A 194    3.663  29.948  11.521  1.00 37.53  A C
ATOM 1258  CE  LYS A 194    4.045  29.470  10.123  1.00 39.74  A C
ATOM 1259  NZ  LYS A 194    3.984  27.993   9.954  1.00 41.23  A N
ATOM 1260  C   LYS A 194    4.546  34.152  12.494  1.00 39.86  A C
ATOM 1261  O   LYS A 194    4.521  34.646  11.362  1.00 39.26  A O
ATOM 1262  N   ASP A 195    5.631  34.140  13.266  1.00 41.38  A N
ATOM 1263  CA  ASP A 195    6.893  34.731  12.835  1.00 41.25  A C
ATOM 1264  CB  ASP A 195    7.637  35.308  14.033  1.00 42.85  A C
ATOM 1265  CG  ASP A 195    6.919  36.491  14.646  1.00 45.61  A C
ATOM 1266  OD1 ASP A 195    6.904  36.606  15.892  1.00 45.35  A O
ATOM 1267  OD2 ASP A 195    6.379  37.316  13.876  1.00 49.06  A O
ATOM 1268  C   ASP A 195    7.801  33.757  12.111  1.00 41.44  A C
ATOM 1269  O   ASP A 195    8.742  34.176  11.452  1.00 42.15  A O
ATOM 1270  N   THR A 196    7.534  32.461  12.230  1.00 41.74  A N
ATOM 1271  CA  THR A 196    8.372  31.479  11.554  1.00 41.77  A C
ATOM 1272  CB  THR A 196    8.334  30.107  12.269  1.00 42.52  A C
ATOM 1273  OG1 THR A 196    6.978  29.683  12.453  1.00 43.11  A O
ATOM 1274  CG2 THR A 196    9.022  30.207  13.622  1.00 42.93  A C
ATOM 1275  C   THR A 196    7.961  31.321  10.095  1.00 42.68  A C
ATOM 1276  O   THR A 196    6.962  31.887   9.658  1.00 44.35  A O
ATOM 1277  N   VAL A 197    8.729  30.543   9.344  1.00 43.09  A N
ATOM 1278  CA  VAL A 197    8.467  30.337   7.927  1.00 42.66  A C
ATOM 1279  CB  VAL A 197    9.684  29.640   7.259  1.00 43.70  A C
ATOM 1280  CG1 VAL A 197    9.847  28.226   7.815  1.00 43.29  A C
ATOM 1281  CG2 VAL A 197    9.518  29.618   5.747  1.00 42.96  A C
ATOM 1282  C   VAL A 197    7.196  29.544   7.626  1.00 42.78  A C
ATOM 1283  O   VAL A 197    6.746  28.735   8.433  1.00 44.36  A O
ATOM 1284  N   TYR A 198    6.606  29.803   6.461  1.00 42.45  A N
ATOM 1285  CA  TYR A 198    5.404  29.098   6.014  1.00 42.25  A C
ATOM 1286  CB  TYR A 198    4.360  30.086   5.468  1.00 38.12  A C
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FIGURE 1A-24

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ATOM 1287  CG  TYR A 198     3.578  30.826   6.533  1.00 35.12  A C
ATOM 1288  CD1 TYR A 198     2.468  30.242   7.145  1.00 32.85  A C
ATOM 1289  CE1 TYR A 198     1.751  30.912   8.142  1.00 30.42  A C
ATOM 1290  CD2 TYR A 198     3.958  32.105   6.947  1.00 33.80  A C
ATOM 1291  CE2 TYR A 198     3.250  32.782   7.945  1.00 32.07  A C
ATOM 1292  CZ  TYR A 198     2.147  32.178   8.534  1.00 32.62  A C
ATOM 1293  OH  TYR A 198     1.428  32.848   9.502  1.00 35.03  A O
ATOM 1294  C   TYR A 198     5.872  28.178   4.891  1.00 44.22  A C
ATOM 1295  O   TYR A 198     6.731  28.566   4.099  1.00 45.17  A O
ATOM 1296  N   THR A 199     5.327  26.969   4.812  1.00 45.87  A N
ATOM 1297  CA  THR A 199     5.743  26.046   3.760  1.00 48.44  A C
ATOM 1298  CB  THR A 199     6.505  24.844   4.333  1.00 47.60  A C
ATOM 1299  OG1 THR A 199     5.656  24.117   5.231  1.00 48.02  A O
ATOM 1300  CG2 THR A 199     7.743  25.320   5.066  1.00 46.04  A C
ATOM 1301  C   THR A 199     4.574  25.536   2.941  1.00 50.70  A C
ATOM 1302  O   THR A 199     4.741  24.698   2.060  1.00 51.37  A O
ATOM 1303  N   ASP A 200     3.387  26.044   3.241  1.00 52.71  A N
ATOM 1304  CA  ASP A 200     2.194  25.654   2.506  1.00 54.80  A C
ATOM 1305  CB  ASP A 200     1.203  24.944   3.425  1.00 57.40  A C
ATOM 1306  CG  ASP A 200     0.618  25.873   4.473  1.00 60.34  A C
ATOM 1307  OD1 ASP A 200     1.408  26.445   5.261  1.00 60.91  A O
ATOM 1308  OD2 ASP A 200    -0.626  26.032   4.505  1.00 60.97  A O
ATOM 1309  C   ASP A 200     1.559  26.928   1.981  1.00 55.09  A C
ATOM 1310  O   ASP A 200     1.691  27.988   2.590  1.00 55.33  A O
ATOM 1311  N   PHE A 201     0.875  26.825   0.850  1.00 55.23  A N
ATOM 1312  CA  PHE A 201     0.207  27.975   0.266  1.00 54.97  A C
ATOM 1313  CB  PHE A 201     1.225  28.931  -0.359  1.00 54.41  A C
ATOM 1314  CG  PHE A 201     0.605  30.040  -1.171  1.00 52.42  A C
ATOM 1315  CD1 PHE A 201     0.327  29.860  -2.521  1.00 51.29  A C
ATOM 1316  CD2 PHE A 201     0.299  31.264  -0.582  1.00 52.75  A C
ATOM 1317  CE1 PHE A 201    -0.247  30.885  -3.278  1.00 53.19  A C
ATOM 1318  CE2 PHE A 201    -0.274  32.296  -1.328  1.00 52.44  A C
ATOM 1319  CZ  PHE A 201    -0.547  32.104  -2.682  1.00 53.31  A C
ATOM 1320  C   PHE A 201    -0.783  27.525  -0.783  1.00 56.67  A C
ATOM 1321  O   PHE A 201    -0.409  26.901  -1.773  1.00 58.10  A O
ATOM 1322  N   ASP A 202    -2.052  27.839  -0.560  1.00 58.05  A N
ATOM 1323  CA  ASP A 202    -3.086  27.468  -1.502  1.00 59.48  A C
ATOM 1324  CB  ASP A 202    -4.047  26.465  -0.859  1.00 62.49  A C
ATOM 1325  CG  ASP A 202    -4.985  25.832  -1.870  1.00 65.65  A C
ATOM 1326  OD1 ASP A 202    -4.479  25.284  -2.876  1.00 68.35  A O
ATOM 1327  OD2 ASP A 202    -6.220  25.879  -1.660  1.00 66.12  A O
ATOM 1328  C   ASP A 202    -3.829  28.721  -1.943  1.00 58.96  A C
ATOM 1329  O   ASP A 202    -5.023  28.686  -2.220  1.00 58.21  A O
ATOM 1330  N   GLY A 203    -3.106  29.833  -2.004  1.00 58.93  A N
ATOM 1331  CA  GLY A 203    -3.712  31.082  -2.417  1.00 58.91  A C
ATOM 1332  C   GLY A 203    -3.799  31.155  -3.927  1.00 58.64  A C
ATOM 1333  O   GLY A 203    -4.063  30.149  -4.575  1.00 59.68  A O
ATOM 1334  N   THR A 204    -3.583  32.342  -4.485  1.00 57.14  A N
ATOM 1335  CA  THR A 204    -3.626  32.540  -5.930  1.00 55.54  A C
ATOM 1336  CB  THR A 204    -4.418  33.816  -6.286  1.00 54.80  A C
ATOM 1337  OG1 THR A 204    -5.691  33.790  -5.628  1.00 52.27  A O
ATOM 1338  CG2 THR A 204    -4.649  33.900  -7.788  1.00 53.52  A C
ATOM 1339  C   THR A 204    -2.182  32.679  -6.411  1.00 56.19  A C
ATOM 1340  O   THR A 204    -1.474  33.605  -6.001  1.00 56.16  A O
ATOM 1341  N   ARG A 205    -1.749  31.765  -7.278  1.00 55.77  A N
ATOM 1342  CA  ARG A 205    -0.371  31.770  -7.771  1.00 56.34  A C
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FIGURE 1A-25

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ATOM 1343  CB  ARG A 205    -0.170  30.656  -8.807  1.00 56.25  A C
ATOM 1344  CG  ARG A 205     1.293  30.248  -8.941  1.00 58.10  A C
ATOM 1345  CD  ARG A 205     1.521  29.131  -9.956  1.00 57.55  A C
ATOM 1346  NE  ARG A 205     2.942  28.793 -10.058  1.00 56.29  A N
ATOM 1347  CZ  ARG A 205     3.629  28.149  -9.119  1.00 56.06  A C
ATOM 1348  NH1 ARG A 205     3.028  27.763  -8.002  1.00 55.25  A N
ATOM 1349  NH2 ARG A 205     4.923  27.899  -9.291  1.00 54.78  A N
ATOM 1350  C   ARG A 205     0.124  33.101  -8.349  1.00 56.38  A C
ATOM 1351  O   ARG A 205     1.173  33.611  -7.952  1.00 57.42  A O
ATOM 1352  N   VAL A 206    -0.624  33.660  -9.291  1.00 55.34  A N
ATOM 1353  CA  VAL A 206    -0.250  34.921  -9.910  1.00 52.95  A C
ATOM 1354  CB  VAL A 206    -1.334  35.329 -10.962  1.00 53.38  A C
ATOM 1355  CG1 VAL A 206    -1.387  36.837 -11.155  1.00 55.30  A C
ATOM 1356  CG2 VAL A 206    -1.009  34.662 -12.289  1.00 50.83  A C
ATOM 1357  C   VAL A 206     0.000  36.026  -8.873  1.00 50.97  A C
ATOM 1358  O   VAL A 206     0.674  37.009  -9.169  1.00 52.03  A O
ATOM 1359  N   TYR A 207    -0.528  35.855  -7.660  1.00 48.29  A N
ATOM 1360  CA  TYR A 207    -0.336  36.825  -6.567  1.00 45.77  A C
ATOM 1361  CB  TYR A 207    -1.651  37.087  -5.804  1.00 44.52  A C
ATOM 1362  CG  TYR A 207    -2.613  38.094  -6.406  1.00 43.56  A C
ATOM 1363  CD1 TYR A 207    -3.474  37.746  -7.455  1.00 43.38  A C
ATOM 1364  CE1 TYR A 207    -4.384  38.667  -7.980  1.00 42.87  A C
ATOM 1365  CD2 TYR A 207    -2.684  39.392  -5.901  1.00 44.41  A C
ATOM 1366  CE2 TYR A 207    -3.587  40.323  -6.415  1.00 45.21  A C
ATOM 1367  CZ  TYR A 207    -4.438  39.958  -7.454  1.00 46.64  A C
ATOM 1368  OH  TYR A 207    -5.345  40.891  -7.943  1.00 49.10  A O
ATOM 1369  C   TYR A 207     0.700  36.322  -5.538  1.00 44.78  A C
ATOM 1370  O   TYR A 207     0.861  36.929  -4.471  1.00 43.46  A O
ATOM 1371  N   SER A 208     1.381  35.218  -5.847  1.00 42.94  A N
ATOM 1372  CA  SER A 208     2.378  34.637  -4.937  1.00 41.95  A C
ATOM 1373  CB  SER A 208     2.430  33.113  -5.112  1.00 42.07  A C
ATOM 1374  OG  SER A 208     3.050  32.758  -6.341  1.00 44.16  A O
ATOM 1375  C   SER A 208     3.779  35.228  -5.153  1.00 39.97  A C
ATOM 1376  O   SER A 208     4.191  35.498  -6.280  1.00 40.64  A O
ATOM 1377  N   PRO A 209     4.537  35.414  -4.066  1.00 38.50  A N
ATOM 1378  CD  PRO A 209     4.225  35.019  -2.680  1.00 36.25  A C
ATOM 1379  CA  PRO A 209     5.884  35.982  -4.160  1.00 39.03  A C
ATOM 1380  CB  PRO A 209     6.194  36.333  -2.715  1.00 37.44  A C
ATOM 1381  CG  PRO A 209     5.558  35.195  -1.977  1.00 36.18  A C
ATOM 1382  C   PRO A 209     6.941  35.050  -4.775  1.00 40.30  A C
ATOM 1383  O   PRO A 209     6.761  33.837  -4.841  1.00 38.77  A O
ATOM 1384  N   PRO A 210     8.067  35.624  -5.230  1.00 41.29  A N
ATOM 1385  CD  PRO A 210     8.412  37.056  -5.173  1.00 41.34  A C
ATOM 1386  CA  PRO A 210     9.153  34.849  -5.836  1.00 41.56  A C
ATOM 1387  CB  PRO A 210    10.230  35.905  -6.096  1.00 41.58  A C
ATOM 1388  CG  PRO A 210     9.451  37.172  -6.253  1.00 42.62  A C
ATOM 1389  C   PRO A 210     9.660  33.730  -4.915  1.00 41.99  A C
ATOM 1390  O   PRO A 210     9.893  32.610  -5.367  1.00 42.50  A O
ATOM 1391  N   GLU A 211     9.832  34.041  -3.629  1.00 41.80  A N
ATOM 1392  CA  GLU A 211    10.316  33.063  -2.656  1.00 41.56  A C
ATOM 1393  CB  GLU A 211    10.460  33.694  -1.265  1.00 40.51  A C
ATOM 1394  CG  GLU A 211     9.190  34.343  -0.729  1.00 40.35  A C
ATOM 1395  CD  GLU A 211     9.050  35.790  -1.175  1.00 40.59  A C
ATOM 1396  OE1 GLU A 211     9.462  36.108  -2.310  1.00 40.81  A O
ATOM 1397  OE2 GLU A 211     8.524  36.611  -0.396  1.00 38.17  A O
ATOM 1398  C   GLU A 211     9.420  31.833  -2.558  1.00 42.93  A C
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FIGURE 1A-26

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ATOM 1399  O   GLU A 211     9.881  30.765  -2.179  1.00 43.46  A O
ATOM 1400  N   TRP A 212     8.140  31.968  -2.875  1.00 43.87  A N
ATOM 1401  CA  TRP A 212     7.268  30.804  -2.816  1.00 45.89  A C
ATOM 1402  CB  TRP A 212     5.799  31.209  -2.678  1.00 44.93  A C
ATOM 1403  CG  TRP A 212     4.844  30.087  -3.012  1.00 45.90  A C
ATOM 1404  CD2 TRP A 212     4.615  28.891  -2.249  1.00 45.90  A C
ATOM 1405  CE2 TRP A 212     3.644  28.132  -2.943  1.00 46.11  A C
ATOM 1406  CE3 TRP A 212     5.138  28.387  -1.048  1.00 44.35  A C
ATOM 1407  CD1 TRP A 212     4.028  30.003  -4.106  1.00 45.66  A C
ATOM 1408  NE1 TRP A 212     3.303  28.835  -4.070  1.00 46.67  A N
ATOM 1409  CZ2 TRP A 212     3.182  26.894  -2.476  1.00 44.29  A C
ATOM 1410  CZ3 TRP A 212     4.679  27.154  -0.582  1.00 43.39  A C
ATOM 1411  CH2 TRP A 212     3.709  26.423  -1.298  1.00 43.70  A C
ATOM 1412  C   TRP A 212     7.442  29.989  -4.087  1.00 48.49  A C
ATOM 1413  O   TRP A 212     7.482  28.759  -4.045  1.00 49.01  A O
ATOM 1414  N   ILE A 213     7.536  30.687  -5.215  1.00 50.82  A N
ATOM 1415  CA  ILE A 213     7.697  30.050  -6.518  1.00 53.85  A C
ATOM 1416  CB  ILE A 213     7.704  31.113  -7.658  1.00 54.33  A C
ATOM 1417  CG2 ILE A 213     7.812  30.441  -9.009  1.00 54.52  A C
ATOM 1418  CG1 ILE A 213     6.424  31.950  -7.616  1.00 55.71  A C
ATOM 1419  CD1 ILE A 213     5.150  31.170  -7.875  1.00 57.18  A C
ATOM 1420  C   ILE A 213     9.007  29.260  -6.588  1.00 55.61  A C
ATOM 1421  O   ILE A 213     9.045  28.149  -7.117  1.00 56.62  A O
ATOM 1422  N   ARG A 214    10.070  29.829  -6.028  1.00 57.11  A N
ATOM 1423  CA  ARG A 214    11.392  29.212  -6.063  1.00 58.32  A C
ATOM 1424  CB  ARG A 214    12.456  30.297  -6.201  1.00 59.98  A C
ATOM 1425  CG  ARG A 214    12.298  31.166  -7.427  1.00 63.19  A C
ATOM 1426  CD  ARG A 214    13.450  32.142  -7.533  1.00 65.99  A C
ATOM 1427  NE  ARG A 214    14.730  31.458  -7.393  1.00 69.47  A N
ATOM 1428  CZ  ARG A 214    15.909  32.030  -7.611  1.00 72.34  A C
ATOM 1429  NH1 ARG A 214    15.968  33.304  -7.986  1.00 72.66  A N
ATOM 1430  NH2 ARG A 214    17.029  31.332  -7.449  1.00 73.16  A N
ATOM 1431  C   ARG A 214    11.804  28.292  -4.920  1.00 58.28  A C
ATOM 1432  O   ARG A 214    12.529  27.331  -5.145  1.00 59.11  A O
ATOM 1433  N   TYR A 215    11.363  28.579  -3.699  1.00 57.89  A N
ATOM 1434  CA  TYR A 215    11.758  27.758  -2.559  1.00 56.71  A C
ATOM 1435  CB  TYR A 215    12.629  28.590  -1.617  1.00 55.81  A C
ATOM 1436  CG  TYR A 215    13.732  29.350  -2.324  1.00 57.72  A C
ATOM 1437  CD1 TYR A 215    14.696  28.680  -3.084  1.00 58.14  A C
ATOM 1438  CE1 TYR A 215    15.706  29.378  -3.751  1.00 58.16  A C
ATOM 1439  CD2 TYR A 215    13.807  30.741  -2.247  1.00 58.08  A C
ATOM 1440  CE2 TYR A 215    14.814  31.449  -2.909  1.00 58.25  A C
ATOM 1441  CZ  TYR A 215    15.757  30.761  -3.659  1.00 58.77  A C
ATOM 1442  OH  TYR A 215    16.745  31.456  -4.320  1.00 59.43  A O
ATOM 1443  C   TYR A 215    10.596  27.160  -1.775  1.00 56.42  A C
ATOM 1444  O   TYR A 215    10.797  26.503  -0.752  1.00 57.33  A O
ATOM 1445  N   HIS A 216     9.382  27.370  -2.259  1.00 55.65  A N
ATOM 1446  CA  HIS A 216     8.208  26.865  -1.566  1.00 55.76  A C
ATOM 1447  CB  HIS A 216     8.107  25.343  -1.693  1.00 59.30  A C
ATOM 1448  CG  HIS A 216     7.788  24.876  -3.080  1.00 64.70  A C
ATOM 1449  CD2 HIS A 216     6.614  24.509  -3.648  1.00 66.31  A C
ATOM 1450  ND1 HIS A 216     8.737  24.803  -4.079  1.00 66.85  A N
ATOM 1451  CE1 HIS A 216     8.160  24.413  -5.203  1.00 67.73  A C
ATOM 1452  NE2 HIS A 216     6.873  24.229  -4.969  1.00 68.11  A N
ATOM 1453  C   HIS A 216     8.224  27.266  -0.096  1.00 53.64  A C
ATOM 1454  O   HIS A 216     7.912  26.466   0.779  1.00 53.38  A O
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FIGURE 1A-27

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ATOM 1455  N   ARG A 217     8.607  28.511   0.165  1.00 51.34  A N
ATOM 1456  CA  ARG A 217     8.627  29.050   1.521  1.00 49.68  A C
ATOM 1457  CB  ARG A 217     9.850  28.540   2.299  1.00 51.09  A C
ATOM 1458  CG  ARG A 217    11.187  28.756   1.620  1.00 54.13  A C
ATOM 1459  CD  ARG A 217    12.275  27.885   2.262  1.00 56.02  A C
ATOM 1460  NE  ARG A 217    12.679  28.347   3.590  1.00 57.63  A N
ATOM 1461  CZ  ARG A 217    12.726  27.577   4.676  1.00 57.75  A C
ATOM 1462  NH1 ARG A 217    12.386  26.293   4.608  1.00 56.48  A N
ATOM 1463  NH2 ARG A 217    13.125  28.091   5.833  1.00 57.35  A N
ATOM 1464  C   ARG A 217     8.595  30.582   1.509  1.00 46.90  A C
ATOM 1465  O   ARG A 217     9.125  31.226   0.599  1.00 46.93  A O
ATOM 1466  N   TYR A 218     7.959  31.156   2.524  1.00 43.17  A N
ATOM 1467  CA  TYR A 218     7.839  32.602   2.648  1.00 39.29  A C
ATOM 1468  CB  TYR A 218     6.745  33.117   1.706  1.00 38.39  A C
ATOM 1469  CG  TYR A 218     5.398  32.487   1.975  1.00 35.47  A C
ATOM 1470  CD1 TYR A 218     4.483  33.085   2.841  1.00 34.99  A C
ATOM 1471  CE1 TYR A 218     3.267  32.469   3.141  1.00 33.86  A C
ATOM 1472  CD2 TYR A 218     5.065  31.253   1.413  1.00 36.77  A C
ATOM 1473  CE2 TYR A 218     3.853  30.625   1.710  1.00 36.30  A C
ATOM 1474  CZ  TYR A 218     2.964  31.237   2.567  1.00 36.25  A C
ATOM 1475  OH  TYR A 218     1.762  30.626   2.830  1.00 37.87  A O
ATOM 1476  C   TYR A 218     7.457  32.948   4.068  1.00 38.43  A C
ATOM 1477  O   TYR A 218     7.143  32.068   4.870  1.00 37.63  A O
ATOM 1478  N   HIS A 219     7.484  34.241   4.371  1.00 37.53  A N
ATOM 1479  CA  HIS A 219     7.092  34.721   5.681  1.00 36.66  A C
ATOM 1480  CB  HIS A 219     8.235  35.511   6.322  1.00 39.29  A C
ATOM 1481  CG  HIS A 219     9.345  34.637   6.817  1.00 41.62  A C
ATOM 1482  CD2 HIS A 219     9.666  34.227   8.067  1.00 42.15  A C
ATOM 1483  ND1 HIS A 219    10.214  33.986   5.967  1.00 42.93  A N
ATOM 1484  CE1 HIS A 219    11.019  33.211   6.673  1.00 42.13  A C
ATOM 1485  NE2 HIS A 219    10.706  33.338   7.949  1.00 42.12  A N
ATOM 1486  C   HIS A 219     5.814  35.554   5.533  1.00 35.29  A C
ATOM 1487  O   HIS A 219     5.547  36.117   4.474  1.00 32.86  A O
ATOM 1488  N   GLY A 220     5.028  35.606   6.602  1.00 33.97  A N
ATOM 1489  CA  GLY A 220     3.753  36.300   6.577  1.00 34.01  A C
ATOM 1490  C   GLY A 220     3.662  37.722   6.068  1.00 34.47  A C
ATOM 1491  O   GLY A 220     3.120  37.990   5.001  1.00 33.07  A O
ATOM 1492  N   ARG A 221     4.199  38.641   6.849  1.00 35.68  A N
ATOM 1493  CA  ARG A 221     4.152  40.047   6.527  1.00 35.47  A C
ATOM 1494  CB  ARG A 221     4.778  40.821   7.680  1.00 38.94  A C
ATOM 1495  CG  ARG A 221     4.218  40.383   9.033  1.00 45.41  A C
ATOM 1496  CD  ARG A 221     4.659  41.299  10.167  1.00 50.82  A C
ATOM 1497  NE  ARG A 221     4.134  40.871  11.466  1.00 54.97  A N
ATOM 1498  CZ  ARG A 221     4.514  39.764  12.103  1.00 57.35  A C
ATOM 1499  NH1 ARG A 221     5.426  38.960  11.560  1.00 56.85  A N
ATOM 1500  NH2 ARG A 221     3.996  39.467  13.293  1.00 57.68  A N
ATOM 1501  C   ARG A 221     4.769  40.456   5.195  1.00 34.82  A C
ATOM 1502  O   ARG A 221     4.202  41.294   4.490  1.00 35.58  A O
ATOM 1503  N   SER A 222     5.906  39.870   4.832  1.00 32.20  A N
ATOM 1504  CA  SER A 222     6.547  40.236   3.576  1.00 31.50  A C
ATOM 1505  CB  SER A 222     8.034  39.861   3.592  1.00 30.38  A C
ATOM 1506  OG  SER A 222     8.215  38.469   3.749  1.00 35.60  A O
ATOM 1507  C   SER A 222     5.857  39.629   2.352  1.00 31.01  A C
ATOM 1508  O   SER A 222     5.859  40.224   1.273  1.00 30.92  A O
ATOM 1509  N   ALA A 223     5.269  38.449   2.507  1.00 30.00  A N
ATOM 1510  CA  ALA A 223     4.558  37.849   1.386  1.00 30.04  A C
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FIGURE 1A-28

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ATOM 1511  CB  ALA A 223     4.157  36.405   1.698  1.00 26.80   A C
ATOM 1512  C   ALA A 223     3.313  38.709   1.181  1.00 30.81   A C
ATOM 1513  O   ALA A 223     2.960  39.059   0.047  1.00 32.87   A O
ATOM 1514  N   ALA A 224     2.665  39.069   2.286  1.00 28.37   A N
ATOM 1515  CA  ALA A 224     1.461  39.888   2.214  1.00 28.82   A C
ATOM 1516  CB  ALA A 224     0.948  40.189   3.610  1.00 25.83   A C
ATOM 1517  C   ALA A 224     1.738  41.191   1.465  1.00 29.93   A C
ATOM 1518  O   ALA A 224     0.941  41.625   0.628  1.00 30.60   A O
ATOM 1519  N   VAL A 225     2.879  41.806   1.759  1.00 29.82   A N
ATOM 1520  CA  VAL A 225     3.244  43.060   1.117  1.00 27.98   A C
ATOM 1521  CB  VAL A 225     4.563  43.612   1.702  1.00 27.45   A C
ATOM 1522  CG1 VAL A 225     5.176  44.649   0.761  1.00 25.52   A C
ATOM 1523  CG2 VAL A 225     4.283  44.226   3.072  1.00 28.24   A C
ATOM 1524  C   VAL A 225     3.379  42.881  -0.381  1.00 28.65   A C
ATOM 1525  O   VAL A 225     2.997  43.761  -1.150  1.00 29.94   A O
ATOM 1526  N   TRP A 226     3.920  41.737  -0.794  1.00 29.04   A N
ATOM 1527  CA  TRP A 226     4.093  41.450  -2.214  1.00 28.73   A C
ATOM 1528  CB  TRP A 226     4.854  40.123  -2.402  1.00 26.66   A C
ATOM 1529  CG  TRP A 226     4.825  39.614  -3.806  1.00 26.75   A C
ATOM 1530  CD2 TRP A 226     5.818  39.825  -4.816  1.00 25.91   A C
ATOM 1531  CE2 TRP A 226     5.336  39.230  -6.009  1.00 26.88   A C
ATOM 1532  CE3 TRP A 226     7.070  40.455  -4.831  1.00 26.80   A C
ATOM 1533  CD1 TRP A 226     3.808  38.911  -4.410  1.00 26.73   A C
ATOM 1534  NE1 TRP A 226     4.109  38.680  -5.734  1.00 26.97   A N
ATOM 1535  CZ2 TRP A 226     6.067  39.252  -7.208  1.00 25.75   A C
ATOM 1536  CZ3 TRP A 226     7.793  40.473  -6.023  1.00 27.87   A C
ATOM 1537  CH2 TRP A 226     7.287  39.873  -7.194  1.00 25.98   A C
ATOM 1538  C   TRP A 226     2.741  41.405  -2.936  1.00 28.31   A C
ATOM 1539  O   TRP A 226     2.586  41.998  -4.000  1.00 30.20   A O
ATOM 1540  N   SER A 227     1.765  40.710  -2.357  1.00 27.18   A N
ATOM 1541  CA  SER A 227     0.445  40.620  -2.975  1.00 28.89   A C
ATOM 1542  CB  SER A 227    -0.439  39.631  -2.201  1.00 28.07   A C
ATOM 1543  OG  SER A 227    -0.852  40.163  -0.953  1.00 31.28   A O
ATOM 1544  C   SER A 227    -0.191  42.018  -2.987  1.00 29.43   A C
ATOM 1545  O   SER A 227    -0.969  42.362  -3.877  1.00 28.11   A O
ATOM 1546  N   LEU A 228     0.155  42.822  -1.990  1.00 29.44   A N
ATOM 1547  CA  LEU A 228    -0.352  44.182  -1.903  1.00 30.04   A C
ATOM 1548  CB  LEU A 228     0.135  44.834  -0.609  1.00 31.55   A C
ATOM 1549  CG  LEU A 228    -0.884  45.233   0.463  1.00 33.80   A C
ATOM 1550  CD1 LEU A 228    -2.235  44.550   0.241  1.00 32.29   A C
ATOM 1551  CD2 LEU A 228    -0.297  44.886   1.837  1.00 33.43   A C
ATOM 1552  C   LEU A 228     0.185  44.942  -3.108  1.00 29.75   A C
ATOM 1553  O   LEU A 228    -0.479  45.825  -3.659  1.00 28.67   A O
ATOM 1554  N   GLY A 229     1.396  44.578  -3.518  1.00 29.14   A N
ATOM 1555  CA  GLY A 229     2.007  45.225  -4.667  1.00 29.41   A C
ATOM 1556  C   GLY A 229     1.317  44.840  -5.969  1.00 28.94   A C
ATOM 1557  O   GLY A 229     1.166  45.668  -6.871  1.00 29.04   A O
ATOM 1558  N   ILE A 230     0.907  43.578  -6.068  1.00 29.31   A N
ATOM 1559  CA  ILE A 230     0.216  43.080  -7.255  1.00 29.40   A C
ATOM 1560  CB  ILE A 230    -0.023  41.567  -7.170  1.00 29.10   A C
ATOM 1561  CG2 ILE A 230    -0.705  41.086  -8.429  1.00 28.94   A C
ATOM 1562  CG1 ILE A 230     1.304  40.831  -6.977  1.00 30.50   A C
ATOM 1563  CD1 ILE A 230     2.237  40.870  -8.191  1.00 30.11   A C
ATOM 1564  C   ILE A 230    -1.143  43.774  -7.332  1.00 29.22   A C
ATOM 1565  O   ILE A 230    -1.561  44.248  -8.388  1.00 27.30   A O
ATOM 1566  N   LEU A 231    -1.819  43.834  -6.189  1.00 29.38   A N
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FIGURE 1A-29

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ATOM 1567  CA  LEU A 231    -3.126  44.473  -6.099  1.00 29.78  A C
ATOM 1568  CB  LEU A 231    -3.626  44.444  -4.647  1.00 28.18  A C
ATOM 1569  CG  LEU A 231    -4.932  45.202  -4.390  1.00 30.16  A C
ATOM 1570  CD1 LEU A 231    -6.073  44.519  -5.138  1.00 27.14  A C
ATOM 1571  CD2 LEU A 231    -5.220  45.268  -2.896  1.00 28.35  A C
ATOM 1572  C   LEU A 231    -3.069  45.920  -6.591  1.00 29.76  A C
ATOM 1573  O   LEU A 231    -3.856  46.322  -7.441  1.00 30.72  A O
ATOM 1574  N   LEU A 232    -2.126  46.692  -6.055  1.00 31.37  A N
ATOM 1575  CA  LEU A 232    -1.966  48.093  -6.419  1.00 29.70  A C
ATOM 1576  CB  LEU A 232    -0.766  48.708  -5.690  1.00 28.80  A C
ATOM 1577  CG  LEU A 232    -0.892  50.183  -5.255  1.00 33.43  A C
ATOM 1578  CD1 LEU A 232     0.485  50.814  -5.269  1.00 28.62  A C
ATOM 1579  CD2 LEU A 232    -1.837  50.977  -6.173  1.00 28.98  A C
ATOM 1580  C   LEU A 232    -1.781  48.251  -7.923  1.00 30.14  A C
ATOM 1581  O   LEU A 232    -2.409  49.113  -8.550  1.00 31.91  A O
ATOM 1582  N   TYR A 233    -0.923  47.424  -8.506  1.00 28.82  A N
ATOM 1583  CA  TYR A 233    -0.674  47.500  -9.938  1.00 29.03  A C
ATOM 1584  CB  TYR A 233     0.417  46.495 -10.341  1.00 28.69  A C
ATOM 1585  CG  TYR A 233     0.758  46.498 -11.818  1.00 29.97  A C
ATOM 1586  CD1 TYR A 233    -0.056  45.842 -12.737  1.00 28.70  A C
ATOM 1587  CE1 TYR A 233     0.224  45.865 -14.100  1.00 29.68  A C
ATOM 1588  CD2 TYR A 233     1.879  47.183 -12.302  1.00 30.67  A C
ATOM 1589  CE2 TYR A 233     2.173  47.217 -13.674  1.00 30.89  A C
ATOM 1590  CZ  TYR A 233     1.331  46.552 -14.565  1.00 31.96  A C
ATOM 1591  OH  TYR A 233     1.567  46.588 -15.920  1.00 31.46  A O
ATOM 1592  C   TYR A 233    -1.985  47.206 -10.658  1.00 29.59  A C
ATOM 1593  O   TYR A 233    -2.362  47.914 -11.590  1.00 31.47  A O
ATOM 1594  N   ASP A 234    -2.683  46.172 -10.198  1.00 29.70  A N
ATOM 1595  CA  ASP A 234    -3.964  45.767 -10.768  1.00 31.81  A C
ATOM 1596  CB  ASP A 234    -4.596  44.675  -9.911  1.00 33.38  A C
ATOM 1597  CG  ASP A 234    -5.845  44.081 -10.540  1.00 36.99  A C
ATOM 1598  OD1 ASP A 234    -6.751  43.694  -9.776  1.00 41.87  A O
ATOM 1599  OD2 ASP A 234    -5.925  43.980 -11.782  1.00 37.30  A O
ATOM 1600  C   ASP A 234    -4.912  46.957 -10.818  1.00 33.23  A C
ATOM 1601  O   ASP A 234    -5.601  47.165 -11.815  1.00 32.83  A O
ATOM 1602  N   MET A 235    -4.937  47.734  -9.735  1.00 33.37  A N
ATOM 1603  CA  MET A 235    -5.799  48.905  -9.646  1.00 33.84  A C
ATOM 1604  CB  MET A 235    -5.808  49.469  -8.216  1.00 34.04  A C
ATOM 1605  CG  MET A 235    -6.643  48.661  -7.231  1.00 35.41  A C
ATOM 1606  SD  MET A 235    -6.847  49.482  -5.637  1.00 38.92  A S
ATOM 1607  CE  MET A 235    -5.328  49.186  -4.882  1.00 36.56  A C
ATOM 1608  C   MET A 235    -5.455  50.032 -10.610  1.00 33.28  A C
ATOM 1609  O   MET A 235    -6.335  50.583 -11.248  1.00 33.36  A O
ATOM 1610  N   VAL A 236    -4.184  50.381 -10.735  1.00 33.08  A N
ATOM 1611  CA  VAL A 236    -3.848  51.489 -11.611  1.00 31.48  A C
ATOM 1612  CB  VAL A 236    -2.711  52.323 -10.992  1.00 29.51  A C
ATOM 1613  CG1 VAL A 236    -3.136  52.772  -9.593  1.00 26.83  A C
ATOM 1614  CG2 VAL A 236    -1.428  51.525 -10.931  1.00 26.01  A C
ATOM 1615  C   VAL A 236    -3.538  51.153 -13.069  1.00 33.38  A C
ATOM 1616  O   VAL A 236    -3.406  52.055 -13.891  1.00 33.89  A O
ATOM 1617  N   CYS A 237    -3.444  49.867 -13.388  1.00 34.36  A N
ATOM 1618  CA  CYS A 237    -3.173  49.425 -14.754  1.00 37.16  A C
ATOM 1619  CB  CYS A 237    -1.901  48.571 -14.808  1.00 36.82  A C
ATOM 1620  SG  CYS A 237    -0.368  49.510 -14.603  1.00 40.55  A S
ATOM 1621  C   CYS A 237    -4.352  48.608 -15.286  1.00 40.02  A C
ATOM 1622  O   CYS A 237    -4.461  48.354 -16.492  1.00 39.93  A O
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FIGURE 1A-30

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ATOM 1623  N   GLY A 238   -5.229  48.192 -14.377  1.00 41.45  A N
ATOM 1624  CA  GLY A 238   -6.392  47.421 -14.769  1.00 42.44  A C
ATOM 1625  C   GLY A 238   -6.103  45.969 -15.085  1.00 43.65  A C
ATOM 1626  O   GLY A 238   -6.838  45.343 -15.837  1.00 44.52  A O
ATOM 1627  N   ASP A 239   -5.040  45.427 -14.505  1.00 44.83  A N
ATOM 1628  CA  ASP A 239   -4.672  44.040 -14.740  1.00 45.73  A C
ATOM 1629  CB  ASP A 239   -4.430  43.828 -16.231  1.00 49.44  A C
ATOM 1630  CG  ASP A 239   -4.775  42.431 -16.681  1.00 52.88  A C
ATOM 1631  OD1 ASP A 239   -4.811  42.209 -17.914  1.00 54.21  A O
ATOM 1632  OD2 ASP A 239   -5.010  41.560 -15.807  1.00 54.96  A O
ATOM 1633  C   ASP A 239   -3.405  43.708 -13.954  1.00 45.17  A C
ATOM 1634  O   ASP A 239   -2.605  44.597 -13.667  1.00 43.18  A O
ATOM 1635  N   ILE A 240   -3.224  42.438 -13.600  1.00 44.12  A N
ATOM 1636  CA  ILE A 240   -2.041  42.046 -12.851  1.00 44.11  A C
ATOM 1637  CB  ILE A 240   -2.163  40.621 -12.252  1.00 45.03  A C
ATOM 1638  CG2 ILE A 240   -3.298  40.602 -11.234  1.00 43.74  A C
ATOM 1639  CG1 ILE A 240   -2.371  39.574 -13.350  1.00 46.17  A C
ATOM 1640  CD1 ILE A 240   -3.770  39.540 -13.934  1.00 49.52  A C
ATOM 1641  C   ILE A 240   -0.814  42.141 -13.741  1.00 44.06  A C
ATOM 1642  O   ILE A 240   -0.909  42.026 -14.958  1.00 44.62  A O
ATOM 1643  N   PRO A 241    0.358  42.366 -13.138  1.00 44.08  A N
ATOM 1644  CD  PRO A 241    0.526  42.567 -11.686  1.00 44.01  A C
ATOM 1645  CA  PRO A 241    1.645  42.501 -13.826  1.00 45.17  A C
ATOM 1646  CB  PRO A 241    2.501  43.201 -12.781  1.00 44.01  A C
ATOM 1647  CG  PRO A 241    2.040  42.526 -11.519  1.00 43.19  A C
ATOM 1648  C   PRO A 241    2.325  41.233 -14.335  1.00 46.15  A C
ATOM 1649  O   PRO A 241    2.969  41.255 -15.378  1.00 46.04  A O
ATOM 1650  N   PHE A 242    2.194  40.139 -13.595  1.00 47.32  A N
ATOM 1651  CA  PHE A 242    2.845  38.894 -13.971  1.00 47.77  A C
ATOM 1652  CB  PHE A 242    3.797  38.458 -12.859  1.00 44.58  A C
ATOM 1653  CG  PHE A 242    4.706  39.549 -12.383  1.00 43.74  A C
ATOM 1654  CD1 PHE A 242    5.501  40.254 -13.284  1.00 43.12  A C
ATOM 1655  CD2 PHE A 242    4.783  39.865 -11.032  1.00 43.56  A C
ATOM 1656  CE1 PHE A 242    6.362  41.260 -12.846  1.00 42.67  A C
ATOM 1657  CE2 PHE A 242    5.643  40.870 -10.577  1.00 42.21  A C
ATOM 1658  CZ  PHE A 242    6.434  41.568 -11.486  1.00 43.87  A C
ATOM 1659  C   PHE A 242    1.864  37.773 -14.250  1.00 50.58  A C
ATOM 1660  O   PHE A 242    0.860  37.621 -13.551  1.00 50.52  A O
ATOM 1661  N   GLU A 243    2.174  36.979 -15.269  1.00 53.46  A N
ATOM 1662  CA  GLU A 243    1.329  35.861 -15.650  1.00 57.46  A C
ATOM 1663  CB  GLU A 243    0.872  36.031 -17.101  1.00 60.72  A C
ATOM 1664  CG  GLU A 243   -0.209  35.057 -17.530  1.00 67.16  A C
ATOM 1665  CD  GLU A 243   -1.402  35.048 -16.574  1.00 71.20  A C
ATOM 1666  OE1 GLU A 243   -2.021  36.120 -16.366  1.00 72.18  A O
ATOM 1667  OE2 GLU A 243   -1.718  33.963 -16.032  1.00 72.59  A O
ATOM 1668  C   GLU A 243    2.064  34.527 -15.475  1.00 58.57  A C
ATOM 1669  O   GLU A 243    1.479  33.547 -15.009  1.00 59.52  A O
ATOM 1670  N   HIS A 244    3.346  34.494 -15.831  1.00 58.69  A N
ATOM 1671  CA  HIS A 244    4.132  33.268 -15.711  1.00 59.32  A C
ATOM 1672  CB  HIS A 244    4.823  32.951 -17.041  1.00 61.16  A C
ATOM 1673  CG  HIS A 244    3.889  32.923 -18.208  1.00 64.11  A C
ATOM 1674  CD2 HIS A 244    3.015  31.977 -18.628  1.00 65.01  A C
ATOM 1675  ND1 HIS A 244    3.733  33.994 -19.062  1.00 65.34  A N
ATOM 1676  CE1 HIS A 244    2.802  33.712 -19.957  1.00 65.53  A C
ATOM 1677  NE2 HIS A 244    2.349  32.494 -19.714  1.00 66.38  A N
ATOM 1678  C   HIS A 244    5.176  33.318 -14.598  1.00 58.34  A C
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FIGURE 1A-31

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ATOM 1679  O   HIS A 244     5.700  34.378 -14.258  1.00 57.57  A O
ATOM 1680  N   ASP A 245     5.477  32.149 -14.044  1.00 57.24  A N
ATOM 1681  CA  ASP A 245     6.449  32.023 -12.969  1.00 55.63  A C
ATOM 1682  CB  ASP A 245     6.726  30.544 -12.699  1.00 55.72  A C
ATOM 1683  CG  ASP A 245     5.507  29.808 -12.167  1.00 57.48  A C
ATOM 1684  OD1 ASP A 245     4.402  30.392 -12.172  1.00 58.01  A O
ATOM 1685  OD2 ASP A 245     5.651  28.640 -11.743  1.00 57.36  A O
ATOM 1686  C   ASP A 245     7.757  32.749 -13.265  1.00 54.41  A C
ATOM 1687  O   ASP A 245     8.339  33.373 -12.378  1.00 53.46  A O
ATOM 1688  N   GLU A 246     8.218  32.669 -14.510  1.00 54.03  A N
ATOM 1689  CA  GLU A 246     9.466  33.327 -14.905  1.00 53.90  A C
ATOM 1690  CB  GLU A 246     9.774  33.088 -16.393  1.00 54.95  A C
ATOM 1691  CG  GLU A 246     9.805  31.642 -16.837  1.00 59.76  A C
ATOM 1692  CD  GLU A 246     8.445  30.969 -16.756  1.00 63.31  A C
ATOM 1693  OE1 GLU A 246     7.441  31.593 -17.162  1.00 64.50  A O
ATOM 1694  OE2 GLU A 246     8.382  29.809 -16.295  1.00 65.65  A O
ATOM 1695  C   GLU A 246     9.376  34.835 -14.668  1.00 52.01  A C
ATOM 1696  O   GLU A 246    10.337  35.464 -14.224  1.00 51.71  A O
ATOM 1697  N   GLU A 247     8.221  35.412 -14.988  1.00 50.73  A N
ATOM 1698  CA  GLU A 247     8.011  36.845 -14.814  1.00 49.15  A C
ATOM 1699  CB  GLU A 247     6.687  37.277 -15.437  1.00 50.68  A C
ATOM 1700  CG  GLU A 247     6.630  37.180 -16.942  1.00 52.81  A C
ATOM 1701  CD  GLU A 247     5.229  37.414 -17.454  1.00 55.13  A C
ATOM 1702  OE1 GLU A 247     4.344  36.589 -17.142  1.00 56.25  A O
ATOM 1703  OE2 GLU A 247     5.006  38.423 -18.155  1.00 57.35  A O
ATOM 1704  C   GLU A 247     8.008  37.206 -13.339  1.00 46.35  A C
ATOM 1705  O   GLU A 247     8.549  38.238 -12.951  1.00 45.63  A O
ATOM 1706  N   ILE A 248     7.397  36.359 -12.518  1.00 43.56  A N
ATOM 1707  CA  ILE A 248     7.356  36.619 -11.092  1.00 42.53  A C
ATOM 1708  CB  ILE A 248     6.499  35.567 -10.339  1.00 40.76  A C
ATOM 1709  CG2 ILE A 248     6.545  35.823  -8.826  1.00 37.81  A C
ATOM 1710  CG1 ILE A 248     5.052  35.629 -10.848  1.00 38.01  A C
ATOM 1711  CD1 ILE A 248     4.106  34.691 -10.145  1.00 35.15  A C
ATOM 1712  C   ILE A 248     8.770  36.631 -10.534  1.00 43.86  A C
ATOM 1713  O   ILE A 248     9.134  37.540  -9.791  1.00 42.81  A O
ATOM 1714  N   ILE A 249     9.584  35.646 -10.908  1.00 46.59  A N
ATOM 1715  CA  ILE A 249    10.957  35.607 -10.393  1.00 48.80  A C
ATOM 1716  CB  ILE A 249    11.641  34.216 -10.571  1.00 49.46  A C
ATOM 1717  CG2 ILE A 249    10.817  33.135  -9.893  1.00 48.12  A C
ATOM 1718  CG1 ILE A 249    11.826  33.898 -12.056  1.00 52.41  A C
ATOM 1719  CD1 ILE A 249    12.559  32.582 -12.318  1.00 56.39  A C
ATOM 1720  C   ILE A 249    11.850  36.665 -11.024  1.00 49.20  A C
ATOM 1721  O   ILE A 249    12.844  37.058 -10.420  1.00 48.98  A O
ATOM 1722  N   ARG A 250    11.510  37.125 -12.228  1.00 50.02  A N
ATOM 1723  CA  ARG A 250    12.316  38.158 -12.884  1.00 51.98  A C
ATOM 1724  CB  ARG A 250    11.889  38.345 -14.345  1.00 53.16  A C
ATOM 1725  CG  ARG A 250    13.002  38.077 -15.351  1.00 55.24  A C
ATOM 1726  CD  ARG A 250    13.591  39.345 -15.976  1.00 56.12  A C
ATOM 1727  NE  ARG A 250    12.721  39.887 -17.016  1.00 58.75  A N
ATOM 1728  CZ  ARG A 250    13.050  40.869 -17.858  1.00 60.36  A C
ATOM 1729  NH1 ARG A 250    14.249  41.442 -17.803  1.00 60.35  A N
ATOM 1730  NH2 ARG A 250    12.166  41.284 -18.761  1.00 59.20  A N
ATOM 1731  C   ARG A 250    12.166  39.479 -12.133  1.00 52.30  A C
ATOM 1732  O   ARG A 250    13.118  40.253 -12.010  1.00 51.53  A O
ATOM 1733  N   GLY A 251    10.961  39.726 -11.633  1.00 52.54  A N
ATOM 1734  CA  GLY A 251    10.718  40.942 -10.886  1.00 54.08  A C
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FIGURE 1A-32

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ATOM 1735  C   GLY A 251   10.581  42.195 -11.735  1.00 54.35  A C
ATOM 1736  O   GLY A 251   10.210  43.241 -11.208  1.00 55.96  A O
ATOM 1737  N   GLN A 252   10.890  42.126 -13.028  1.00 53.37  A N
ATOM 1738  CA  GLN A 252   10.754  43.308 -13.881  1.00 51.24  A C
ATOM 1739  CB  GLN A 252   11.314  43.040 -15.279  1.00 54.94  A C
ATOM 1740  CG  GLN A 252   12.797  42.809 -15.314  1.00 60.65  A C
ATOM 1741  CD  GLN A 252   13.554  44.030 -15.770  1.00 63.68  A C
ATOM 1742  OE1 GLN A 252   14.790  44.069 -15.725  1.00 67.10  A O
ATOM 1743  NE2 GLN A 252   12.819  45.039 -16.217  1.00 64.32  A N
ATOM 1744  C   GLN A 252    9.285  43.673 -14.007  1.00 47.89  A C
ATOM 1745  O   GLN A 252    8.456  42.840 -14.372  1.00 47.19  A O
ATOM 1746  N   VAL A 253    8.952  44.915 -13.700  1.00 44.04  A N
ATOM 1747  CA  VAL A 253    7.574  45.336 -13.823  1.00 40.99  A C
ATOM 1748  CB  VAL A 253    6.999  45.787 -12.452  1.00 40.04  A C
ATOM 1749  CG1 VAL A 253    8.108  46.315 -11.590  1.00 42.49  A C
ATOM 1750  CG2 VAL A 253    5.909  46.842 -12.635  1.00 38.06  A C
ATOM 1751  C   VAL A 253    7.467  46.432 -14.867  1.00 39.88  A C
ATOM 1752  O   VAL A 253    8.087  47.489 -14.762  1.00 40.31  A O
ATOM 1753  N   PHE A 254    6.692  46.143 -15.903  1.00 38.47  A N
ATOM 1754  CA  PHE A 254    6.473  47.063 -17.006  1.00 38.09  A C
ATOM 1755  CB  PHE A 254    6.606  46.297 -18.341  1.00 39.78  A C
ATOM 1756  CG  PHE A 254    6.055  47.041 -19.531  1.00 43.02  A C
ATOM 1757  CD1 PHE A 254    4.702  46.941 -19.872  1.00 44.05  A C
ATOM 1758  CD2 PHE A 254    6.871  47.895 -20.273  1.00 43.12  A C
ATOM 1759  CE1 PHE A 254    4.174  47.688 -20.933  1.00 44.40  A C
ATOM 1760  CE2 PHE A 254    6.353  48.646 -21.333  1.00 42.14  A C
ATOM 1761  CZ  PHE A 254    5.005  48.543 -21.661  1.00 43.52  A C
ATOM 1762  C   PHE A 254    5.083  47.693 -16.868  1.00 37.93  A C
ATOM 1763  O   PHE A 254    4.113  47.009 -16.540  1.00 38.43  A O
ATOM 1764  N   PHE A 255    4.983  48.997 -17.101  1.00 37.10  A N
ATOM 1765  CA  PHE A 255    3.693  49.653 -16.995  1.00 37.10  A C
ATOM 1766  CB  PHE A 255    3.835  50.984 -16.257  1.00 35.60  A C
ATOM 1767  CG  PHE A 255    4.100  50.815 -14.796  1.00 34.11  A C
ATOM 1768  CD1 PHE A 255    5.381  50.563 -14.334  1.00 32.58  A C
ATOM 1769  CD2 PHE A 255    3.041  50.801 -13.890  1.00 35.04  A C
ATOM 1770  CE1 PHE A 255    5.605  50.294 -12.995  1.00 34.38  A C
ATOM 1771  CE2 PHE A 255    3.252  50.530 -12.545  1.00 33.03  A C
ATOM 1772  CZ  PHE A 255    4.531  50.275 -12.094  1.00 34.57  A C
ATOM 1773  C   PHE A 255    3.027  49.836 -18.345  1.00 38.35  A C
ATOM 1774  O   PHE A 255    3.570  50.466 -19.248  1.00 39.65  A O
ATOM 1775  N   ARG A 256    1.844  49.256 -18.472  1.00 40.83  A N
ATOM 1776  CA  ARG A 256    1.082  49.309 -19.707  1.00 43.82  A C
ATOM 1777  CB  ARG A 256    0.285  48.013 -19.863  1.00 45.87  A C
ATOM 1778  CG  ARG A 256   -0.735  47.778 -18.759  1.00 47.82  A C
ATOM 1779  CD  ARG A 256   -1.363  46.391 -18.886  1.00 50.28  A C
ATOM 1780  NE  ARG A 256   -0.545  45.342 -18.274  1.00 51.16  A N
ATOM 1781  CZ  ARG A 256   -0.713  44.042 -18.498  1.00 51.86  A C
ATOM 1782  NH1 ARG A 256   -1.662  43.630 -19.328  1.00 51.40  A N
ATOM 1783  NH2 ARG A 256    0.054  43.153 -17.877  1.00 50.88  A N
ATOM 1784  C   ARG A 256    0.134  50.499 -19.698  1.00 43.97  A C
ATOM 1785  O   ARG A 256   -0.531  50.789 -20.686  1.00 43.91  A O
ATOM 1786  N   GLN A 257    0.087  51.183 -18.564  1.00 44.59  A N
ATOM 1787  CA  GLN A 257   -0.778  52.339 -18.385  1.00 44.56  A C
ATOM 1788  CB  GLN A 257   -1.910  51.983 -17.424  1.00 47.73  A C
ATOM 1789  CG  GLN A 257   -2.924  53.075 -17.227  1.00 52.66  A C
ATOM 1790  CD  GLN A 257   -3.963  53.077 -18.319  1.00 55.97  A C
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FIGURE 1A-33

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ATOM 1791  OE1 GLN A 257    -3.641  53.155 -19.506  1.00 60.22   A O
ATOM 1792  NE2 GLN A 257    -5.224  52.989 -17.925  1.00 57.29   A N
ATOM 1793  C   GLN A 257     0.035  53.485 -17.798  1.00 42.63   A C
ATOM 1794  O   GLN A 257     1.106  53.282 -17.237  1.00 41.65   A O
ATOM 1795  N   ARG A 258    -0.487  54.693 -17.915  1.00 41.08   A N
ATOM 1796  CA  ARG A 258     0.197  55.864 -17.389  1.00 39.55   A C
ATOM 1797  CB  ARG A 258    -0.399  57.115 -18.030  1.00 39.54   A C
ATOM 1798  CG  ARG A 258     0.516  58.310 -18.048  1.00 39.65   A C
ATOM 1799  CD  ARG A 258     0.880  58.841 -16.677  1.00 38.97   A C
ATOM 1800  NE  ARG A 258     2.214  59.416 -16.772  1.00 43.61   A N
ATOM 1801  CZ  ARG A 258     2.716  60.334 -15.960  1.00 44.90   A C
ATOM 1802  NH1 ARG A 258     1.990  60.810 -14.956  1.00 44.37   A N
ATOM 1803  NH2 ARG A 258     3.950  60.778 -16.169  1.00 45.57   A N
ATOM 1804  C   ARG A 258     0.030  55.962 -15.871  1.00 37.84   A C
ATOM 1805  O   ARG A 258    -1.084  56.141 -15.401  1.00 38.78   A O
ATOM 1806  N   VAL A 259     1.112  55.843 -15.106  1.00 34.70   A N
ATOM 1807  CA  VAL A 259     1.005  55.977 -13.654  1.00 35.02   A C
ATOM 1808  CB  VAL A 259     0.932  54.574 -12.917  1.00 34.62   A C
ATOM 1809  CG1 VAL A 259     1.000  53.454 -13.911  1.00 35.15   A C
ATOM 1810  CG2 VAL A 259     2.008  54.439 -11.870  1.00 33.47   A C
ATOM 1811  C   VAL A 259     2.137  56.850 -13.110  1.00 34.29   A C
ATOM 1812  O   VAL A 259     3.276  56.781 -13.566  1.00 35.06   A O
ATOM 1813  N   SER A 260     1.810  57.691 -12.141  1.00 32.72   A N
ATOM 1814  CA  SER A 260     2.790  58.604 -11.578  1.00 34.11   A C
ATOM 1815  CB  SER A 260     2.178  59.385 -10.414  1.00 31.50   A C
ATOM 1816  OG  SER A 260     1.709  58.502  -9.412  1.00 32.89   A O
ATOM 1817  C   SER A 260     4.065  57.917 -11.119  1.00 35.22   A C
ATOM 1818  O   SER A 260     4.068  56.731 -10.784  1.00 36.19   A O
ATOM 1819  N   PSR A 261     5.152  58.681 -11.116  1.00 36.27   A N
ATOM 1820  CA  PSR A 261     6.444  58.179 -10.690  1.00 36.55   A C
ATOM 1821  CB  PSR A 261     7.496  59.286 -10.791  1.00 37.30   A C
ATOM 1822  OG  PSR A 261     7.670  59.587 -12.171  1.00 43.48   A O
ATOM 1823  C   PSR A 261     6.349  57.666  -9.258  1.00 36.02   A C
ATOM 1824  O   PSR A 261     6.872  56.610  -8.945  1.00 36.34   A O
ATOM 1825  P   PSR A 261     7.258  60.992 -12.776  1.00 47.24   A P
ATOM 1826  O1  PSR A 261     7.996  62.078 -12.123  1.00 45.73   A O
ATOM 1827  O2  PSR A 261     7.487  61.003 -14.295  1.00 46.52   A O
ATOM 1828  O3  PSR A 261     5.734  61.105 -12.561  1.00 46.41   A O
ATOM 1829  N   GLU A 262     5.666  58.407  -8.394  1.00 37.22   A N
ATOM 1830  CA  GLU A 262     5.521  57.994  -7.002  1.00 39.04   A C
ATOM 1831  CB  GLU A 262     4.757  59.041  -6.205  1.00 43.32   A C
ATOM 1832  CG  GLU A 262     5.432  60.384  -6.172  1.00 50.59   A C
ATOM 1833  CD  GLU A 262     4.782  61.326  -5.186  1.00 57.26   A C
ATOM 1834  OE1 GLU A 262     3.531  61.463  -5.215  1.00 61.12   A O
ATOM 1835  OE2 GLU A 262     5.525  61.935  -4.384  1.00 61.01   A O
ATOM 1836  C   GLU A 262     4.816  56.651  -6.868  1.00 36.91   A C
ATOM 1837  O   GLU A 262     5.218  55.817  -6.061  1.00 37.02   A O
ATOM 1838  N   CYS A 263     3.771  56.443  -7.663  1.00 35.35   A N
ATOM 1839  CA  CYS A 263     3.029  55.187  -7.621  1.00 34.69   A C
ATOM 1840  CB  CYS A 263     1.759  55.282  -8.472  1.00 33.75   A C
ATOM 1841  SG  CYS A 263     0.528  53.987  -8.165  1.00 34.55   A S
ATOM 1842  C   CYS A 263     3.919  54.054  -8.136  1.00 34.61   A C
ATOM 1843  O   CYS A 263     4.013  52.989  -7.509  1.00 33.80   A O
ATOM 1844  N   GLN A 264     4.573  54.277  -9.274  1.00 34.11   A N
ATOM 1845  CA  GLN A 264     5.458  53.253  -9.833  1.00 33.15   A C
ATOM 1846  CB  GLN A 264     6.177  53.760 -11.091  1.00 31.97   A C
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FIGURE 1A-34

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ATOM 1847  CG  GLN A 264     5.340  53.769 -12.367  1.00 32.36  A C
ATOM 1848  CD  GLN A 264     6.202  53.961 -13.616  1.00 33.61  A C
ATOM 1849  OE1 GLN A 264     7.407  53.689 -13.595  1.00 36.85  A O
ATOM 1850  NE2 GLN A 264     5.591  54.407 -14.708  1.00 29.45  A N
ATOM 1851  C   GLN A 264     6.495  52.869  -8.785  1.00 32.22  A C
ATOM 1852  O   GLN A 264     6.847  51.689  -8.636  1.00 32.96  A O
ATOM 1853  N   HIS A 265     6.976  53.863  -8.045  1.00 31.19  A N
ATOM 1854  CA  HIS A 265     7.987  53.597  -7.023  1.00 32.17  A C
ATOM 1855  CB  HIS A 265     8.567  54.909  -6.473  1.00 32.44  A C
ATOM 1856  CG  HIS A 265     9.489  54.719  -5.308  1.00 37.25  A C
ATOM 1857  CD2 HIS A 265    10.842  54.627  -5.244  1.00 37.59  A C
ATOM 1858  ND1 HIS A 265     9.034  54.556  -4.016  1.00 36.63  A N
ATOM 1859  CE1 HIS A 265    10.065  54.371  -3.208  1.00 38.61  A C
ATOM 1860  NE2 HIS A 265    11.173  54.409  -3.928  1.00 38.75  A N
ATOM 1861  C   HIS A 265     7.440  52.737  -5.882  1.00 31.92  A C
ATOM 1862  O   HIS A 265     8.098  51.791  -5.454  1.00 32.05  A O
ATOM 1863  N   LEU A 266     6.243  53.048  -5.390  1.00 29.30  A N
ATOM 1864  CA  LEU A 266     5.689  52.250  -4.313  1.00 29.02  A C
ATOM 1865  CB  LEU A 266     4.365  52.839  -3.830  1.00 27.57  A C
ATOM 1866  CG  LEU A 266     3.602  52.079  -2.731  1.00 25.85  A C
ATOM 1867  CD1 LEU A 266     4.497  51.805  -1.527  1.00 20.26  A C
ATOM 1868  CD2 LEU A 266     2.391  52.914  -2.305  1.00 23.77  A C
ATOM 1869  C   LEU A 266     5.484  50.819  -4.811  1.00 29.60  A C
ATOM 1870  O   LEU A 266     5.880  49.860  -4.149  1.00 28.99  A O
ATOM 1871  N   ILE A 267     4.884  50.679  -5.990  1.00 29.64  A N
ATOM 1872  CA  ILE A 267     4.638  49.364  -6.552  1.00 28.48  A C
ATOM 1873  CB  ILE A 267     4.011  49.469  -7.962  1.00 27.24  A C
ATOM 1874  CG2 ILE A 267     4.034  48.112  -8.656  1.00 26.16  A C
ATOM 1875  CG1 ILE A 267     2.570  49.964  -7.841  1.00 27.71  A C
ATOM 1876  CD1 ILE A 267     1.838  50.139  -9.160  1.00 24.12  A C
ATOM 1877  C   ILE A 267     5.933  48.560  -6.614  1.00 30.34  A C
ATOM 1878  O   ILE A 267     6.012  47.453  -6.078  1.00 31.34  A O
ATOM 1879  N   ARG A 268     6.953  49.117  -7.257  1.00 31.40  A N
ATOM 1880  CA  ARG A 268     8.230  48.420  -7.371  1.00 31.84  A C
ATOM 1881  CB  ARG A 268     9.218  49.259  -8.183  1.00 32.59  A C
ATOM 1882  CG  ARG A 268     8.901  49.200  -9.665  1.00 34.16  A C
ATOM 1883  CD  ARG A 268     9.820  50.053 -10.505  1.00 35.56  A C
ATOM 1884  NE  ARG A 268     9.600  49.767 -11.918  1.00 38.19  A N
ATOM 1885  CZ  ARG A 268     9.287  50.685 -12.827  1.00 38.93  A C
ATOM 1886  NH1 ARG A 268     9.163  51.958 -12.463  1.00 37.34  A N
ATOM 1887  NH2 ARG A 268     9.083  50.329 -14.094  1.00 37.13  A N
ATOM 1888  C   ARG A 268     8.816  48.057  -6.017  1.00 30.74  A C
ATOM 1889  O   ARG A 268     9.395  46.977  -5.850  1.00 30.02  A O
ATOM 1890  N   TRP A 269     8.649  48.948  -5.044  1.00 30.52  A N
ATOM 1891  CA  TRP A 269     9.152  48.700  -3.703  1.00 30.64  A C
ATOM 1892  CB  TRP A 269     8.939  49.945  -2.842  1.00 32.44  A C
ATOM 1893  CG  TRP A 269     9.695  49.942  -1.550  1.00 35.34  A C
ATOM 1894  CD2 TRP A 269     9.566  50.887  -0.482  1.00 35.39  A C
ATOM 1895  CE2 TRP A 269    10.483  50.506   0.527  1.00 35.12  A C
ATOM 1896  CE3 TRP A 269     8.766  52.019  -0.278  1.00 35.66  A C
ATOM 1897  CD1 TRP A 269    10.658  49.048  -1.158  1.00 36.30  A C
ATOM 1898  NE1 TRP A 269    11.135  49.383   0.089  1.00 35.88  A N
ATOM 1899  CZ2 TRP A 269    10.620  51.218   1.723  1.00 35.01  A C
ATOM 1900  CZ3 TRP A 269     8.902  52.728   0.912  1.00 35.51  A C
ATOM 1901  CH2 TRP A 269     9.824  52.324   1.897  1.00 36.86  A C
ATOM 1902  C   TRP A 269     8.441  47.474  -3.105  1.00 30.79  A C
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FIGURE 1A-35

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ATOM 1903  O   TRP A 269    9.096  46.550  -2.609  1.00 30.58  A O
ATOM 1904  N   CYS A 270    7.111  47.453  -3.163  1.00 29.63  A N
ATOM 1905  CA  CYS A 270    6.353  46.308  -2.638  1.00 31.31  A C
ATOM 1906  CB  CYS A 270    4.838  46.507  -2.779  1.00 30.49  A C
ATOM 1907  SG  CYS A 270    4.121  47.771  -1.739  1.00 29.16  A S
ATOM 1908  C   CYS A 270    6.716  45.028  -3.378  1.00 31.37  A C
ATOM 1909  O   CYS A 270    6.647  43.942  -2.808  1.00 31.72  A O
ATOM 1910  N   LEU A 271    7.079  45.154  -4.651  1.00 31.04  A N
ATOM 1911  CA  LEU A 271    7.439  43.982  -5.441  1.00 32.09  A C
ATOM 1912  CB  LEU A 271    6.943  44.133  -6.880  1.00 30.32  A C
ATOM 1913  CG  LEU A 271    5.430  44.282  -7.046  1.00 30.65  A C
ATOM 1914  CD1 LEU A 271    5.080  44.393  -8.526  1.00 29.92  A C
ATOM 1915  CD2 LEU A 271    4.722  43.084  -6.406  1.00 30.95  A C
ATOM 1916  C   LEU A 271    8.941  43.698  -5.443  1.00 32.63  A C
ATOM 1917  O   LEU A 271    9.441  43.022  -6.337  1.00 33.86  A O
ATOM 1918  N   ALA A 272    9.666  44.210  -4.453  1.00 32.88  A N
ATOM 1919  CA  ALA A 272   11.102  43.945  -4.390  1.00 33.73  A C
ATOM 1920  CB  ALA A 272   11.712  44.551  -3.132  1.00 30.62  A C
ATOM 1921  C   ALA A 272   11.288  42.433  -4.389  1.00 34.72  A C
ATOM 1922  O   ALA A 272   10.568  41.709  -3.709  1.00 35.00  A O
ATOM 1923  N   LEU A 273   12.257  41.966  -5.162  1.00 36.82  A N
ATOM 1924  CA  LEU A 273   12.544  40.546  -5.279  1.00 38.18  A C
ATOM 1925  CB  LEU A 273   13.626  40.357  -6.342  1.00 35.60  A C
ATOM 1926  CG  LEU A 273   13.273  39.407  -7.487  1.00 38.06  A C
ATOM 1927  CD1 LEU A 273   11.810  39.531  -7.880  1.00 36.55  A C
ATOM 1928  CD2 LEU A 273   14.172  39.719  -8.670  1.00 35.63  A C
ATOM 1929  C   LEU A 273   12.961  39.902  -3.950  1.00 38.58  A C
ATOM 1930  O   LEU A 273   12.546  38.789  -3.628  1.00 39.68  A O
ATOM 1931  N   ARG A 274   13.780  40.603  -3.181  1.00 39.35  A N
ATOM 1932  CA  ARG A 274   14.236  40.093  -1.897  1.00 42.41  A C
ATOM 1933  CB  ARG A 274   15.628  40.654  -1.582  1.00 46.64  A C
ATOM 1934  CG  ARG A 274   16.320  39.987  -0.409  1.00 54.41  A C
ATOM 1935  CD  ARG A 274   17.568  40.764   0.005  1.00 61.03  A C
ATOM 1936  NE  ARG A 274   18.253  40.144   1.140  1.00 65.54  A N
ATOM 1937  CZ  ARG A 274   19.104  40.781   1.942  1.00 68.54  A C
ATOM 1938  NH1 ARG A 274   19.382  42.066   1.742  1.00 69.86  A N
ATOM 1939  NH2 ARG A 274   19.680  40.133   2.949  1.00 69.00  A N
ATOM 1940  C   ARG A 274   13.231  40.522  -0.824  1.00 41.21  A C
ATOM 1941  O   ARG A 274   12.984  41.708  -0.629  1.00 42.03  A O
ATOM 1942  N   PRO A 275   12.636  39.556  -0.119  1.00 40.69  A N
ATOM 1943  CD  PRO A 275   12.857  38.109  -0.291  1.00 40.83  A C
ATOM 1944  CA  PRO A 275   11.649  39.812   0.935  1.00 40.87  A C
ATOM 1945  CB  PRO A 275   11.548  38.461   1.635  1.00 40.32  A C
ATOM 1946  CG  PRO A 275   11.694  37.504   0.489  1.00 41.14  A C
ATOM 1947  C   PRO A 275   11.967  40.946   1.909  1.00 42.07  A C
ATOM 1948  O   PRO A 275   11.098  41.771   2.209  1.00 41.99  A O
ATOM 1949  N   SER A 276   13.203  40.994   2.403  1.00 41.82  A N
ATOM 1950  CA  SER A 276   13.584  42.030   3.358  1.00 41.94  A C
ATOM 1951  CB  SER A 276   14.918  41.680   4.044  1.00 43.82  A C
ATOM 1952  OG  SER A 276   16.009  41.650   3.136  1.00 45.28  A O
ATOM 1953  C   SER A 276   13.660  43.419   2.735  1.00 41.43  A C
ATOM 1954  O   SER A 276   13.666  44.425   3.456  1.00 42.73  A O
ATOM 1955  N   ASP A 277   13.708  43.487   1.405  1.00 39.45  A N
ATOM 1956  CA  ASP A 277   13.762  44.781   0.721  1.00 39.07  A C
ATOM 1957  CB  ASP A 277   14.435  44.642  -0.645  1.00 40.19  A C
ATOM 1958  CG  ASP A 277   15.953  44.578  -0.556  1.00 40.20  A C
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FIGURE 1A-36

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ATOM 1959  OD1 ASP A 277   16.584  44.085  -1.516  1.00 40.93  A O
ATOM 1960  OD2 ASP A 277   16.516  45.031   0.462  1.00 42.38  A O
ATOM 1961  C   ASP A 277   12.361  45.381   0.528  1.00 39.70  A C
ATOM 1962  O   ASP A 277   12.221  46.481   0.000  1.00 40.28  A O
ATOM 1963  N   ARG A 278   11.324  44.662   0.945  1.00 37.62  A N
ATOM 1964  CA  ARG A 278    9.974  45.181   0.790  1.00 36.84  A C
ATOM 1965  CB  ARG A 278    8.962  44.034   0.718  1.00 32.73  A C
ATOM 1966  CG  ARG A 278    9.117  43.197  -0.540  1.00 31.87  A C
ATOM 1967  CD  ARG A 278    8.243  41.947  -0.541  1.00 29.54  A C
ATOM 1968  NE  ARG A 278    8.814  40.978  -1.469  1.00 31.25  A N
ATOM 1969  CZ  ARG A 278    8.600  39.666  -1.445  1.00 30.79  A C
ATOM 1970  NH1 ARG A 278    7.806  39.122  -0.532  1.00 25.69  A N
ATOM 1971  NH2 ARG A 278    9.222  38.892  -2.325  1.00 30.91  A N
ATOM 1972  C   ARG A 278    9.647  46.102   1.953  1.00 36.76  A C
ATOM 1973  O   ARG A 278   10.227  45.988   3.029  1.00 37.02  A O
ATOM 1974  N   PRO A 279    8.726  47.047   1.743  1.00 35.68  A N
ATOM 1975  CD  PRO A 279    8.012  47.372   0.495  1.00 37.47  A C
ATOM 1976  CA  PRO A 279    8.351  47.973   2.808  1.00 35.02  A C
ATOM 1977  CB  PRO A 279    7.595  49.062   2.057  1.00 35.64  A C
ATOM 1978  CG  PRO A 279    6.898  48.283   0.986  1.00 36.36  A C
ATOM 1979  C   PRO A 279    7.477  47.316   3.858  1.00 35.20  A C
ATOM 1980  O   PRO A 279    6.871  46.270   3.617  1.00 36.51  A O
ATOM 1981  N   THR A 280    7.431  47.936   5.030  1.00 35.39  A N
ATOM 1982  CA  THR A 280    6.584  47.472   6.119  1.00 34.83  A C
ATOM 1983  CB  THR A 280    7.115  47.921   7.498  1.00 36.91  A C
ATOM 1984  OG1 THR A 280    7.189  49.352   7.528  1.00 37.55  A O
ATOM 1985  CG2 THR A 280    8.504  47.348   7.771  1.00 35.19  A C
ATOM 1986  C   THR A 280    5.288  48.234   5.860  1.00 34.91  A C
ATOM 1987  O   THR A 280    5.280  49.189   5.080  1.00 33.92  A O
ATOM 1988  N   PHE A 281    4.200  47.827   6.506  1.00 36.78  A N
ATOM 1989  CA  PHE A 281    2.920  48.507   6.328  1.00 36.78  A C
ATOM 1990  CB  PHE A 281    1.879  47.898   7.250  1.00 37.22  A C
ATOM 1991  CG  PHE A 281    1.576  46.471   6.944  1.00 40.21  A C
ATOM 1992  CD1 PHE A 281    1.235  45.590   7.959  1.00 42.91  A C
ATOM 1993  CD2 PHE A 281    1.627  46.000   5.637  1.00 41.13  A C
ATOM 1994  CE1 PHE A 281    0.950  44.263   7.673  1.00 44.48  A C
ATOM 1995  CE2 PHE A 281    1.344  44.675   5.341  1.00 41.80  A C
ATOM 1996  CZ  PHE A 281    1.005  43.804   6.355  1.00 42.76  A C
ATOM 1997  C   PHE A 281    3.074  49.985   6.642  1.00 37.43  A C
ATOM 1998  O   PHE A 281    2.524  50.840   5.943  1.00 36.72  A O
ATOM 1999  N   GLU A 282    3.839  50.278   7.691  1.00 36.23  A N
ATOM 2000  CA  GLU A 282    4.062  51.647   8.103  1.00 36.89  A C
ATOM 2001  CB  GLU A 282    4.900  51.688   9.386  1.00 38.21  A C
ATOM 2002  CG  GLU A 282    5.187  53.093   9.901  1.00 42.14  A C
ATOM 2003  CD  GLU A 282    6.152  53.104  11.080  1.00 45.10  A C
ATOM 2004  OE1 GLU A 282    7.120  52.313  11.063  1.00 47.22  A O
ATOM 2005  OE2 GLU A 282    5.958  53.913  12.015  1.00 45.12  A O
ATOM 2006  C   GLU A 282    4.754  52.419   6.996  1.00 36.11  A C
ATOM 2007  O   GLU A 282    4.390  53.551   6.703  1.00 35.95  A O
ATOM 2008  N   GLU A 283    5.756  51.810   6.376  1.00 36.13  A N
ATOM 2009  CA  GLU A 283    6.478  52.476   5.299  1.00 37.36  A C
ATOM 2010  CB  GLU A 283    7.709  51.664   4.910  1.00 38.74  A C
ATOM 2011  CG  GLU A 283    8.771  51.649   5.991  1.00 39.19  A C
ATOM 2012  CD  GLU A 283    9.980  50.837   5.602  1.00 40.21  A C
ATOM 2013  OE1 GLU A 283    9.835  49.613   5.416  1.00 39.48  A O
ATOM 2014  OE2 GLU A 283   11.075  51.424   5.479  1.00 43.29  A O
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FIGURE 1A-37

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ATOM 2015  C   GLU A 283     5.602  52.727   4.078  1.00 36.38  A C
ATOM 2016  O   GLU A 283     5.787  53.710   3.373  1.00 38.78  A O
ATOM 2017  N   ILE A 284     4.647  51.839   3.825  1.00 35.00  A N
ATOM 2018  CA  ILE A 284     3.738  52.010   2.701  1.00 32.48  A C
ATOM 2019  CB  ILE A 284     2.900  50.747   2.470  1.00 30.83  A C
ATOM 2020  CG2 ILE A 284     1.720  51.047   1.558  1.00 28.46  A C
ATOM 2021  CG1 ILE A 284     3.784  49.648   1.883  1.00 28.96  A C
ATOM 2022  CD1 ILE A 284     3.081  48.325   1.750  1.00 27.87  A C
ATOM 2023  C   ILE A 284     2.801  53.173   3.004  1.00 33.80  A C
ATOM 2024  O   ILE A 284     2.624  54.080   2.182  1.00 33.93  A O
ATOM 2025  N   GLN A 285     2.212  53.156   4.194  1.00 32.53  A N
ATOM 2026  CA  GLN A 285     1.294  54.217   4.572  1.00 33.24  A C
ATOM 2027  CB  GLN A 285     0.507  53.812   5.826  1.00 32.92  A C
ATOM 2028  CG  GLN A 285    -0.432  52.636   5.552  1.00 30.72  A C
ATOM 2029  CD  GLN A 285    -1.547  52.485   6.574  1.00 31.68  A C
ATOM 2030  OE1 GLN A 285    -1.316  52.075   7.713  1.00 29.72  A O
ATOM 2031  NE2 GLN A 285    -2.769  52.815   6.166  1.00 28.89  A N
ATOM 2032  C   GLN A 285     1.981  55.570   4.746  1.00 34.19  A C
ATOM 2033  O   GLN A 285     1.317  56.606   4.747  1.00 35.02  A O
ATOM 2034  N   ASN A 286     3.307  55.573   4.873  1.00 33.74  A N
ATOM 2035  CA  ASN A 286     4.032  56.834   4.995  1.00 33.86  A C
ATOM 2036  CB  ASN A 286     5.145  56.736   6.050  1.00 33.45  A C
ATOM 2037  CG  ASN A 286     4.633  56.976   7.467  1.00 33.36  A C
ATOM 2038  OD1 ASN A 286     5.122  56.376   8.421  1.00 36.12  A O
ATOM 2039  ND2 ASN A 286     3.659  57.863   7.606  1.00 31.81  A N
ATOM 2040  C   ASN A 286     4.639  57.226   3.651  1.00 35.02  A C
ATOM 2041  O   ASN A 286     5.297  58.256   3.539  1.00 37.55  A O
ATOM 2042  N   HIS A 287     4.428  56.402   2.631  1.00 33.15  A N
ATOM 2043  CA  HIS A 287     4.970  56.700   1.311  1.00 32.89  A C
ATOM 2044  CB  HIS A 287     4.721  55.522   0.358  1.00 29.47  A C
ATOM 2045  CG  HIS A 287     5.468  55.626  -0.936  1.00 28.62  A C
ATOM 2046  CD2 HIS A 287     6.627  55.055  -1.342  1.00 25.27  A C
ATOM 2047  ND1 HIS A 287     5.049  56.426  -1.979  1.00 27.58  A N
ATOM 2048  CE1 HIS A 287     5.915  56.339  -2.972  1.00 24.42  A C
ATOM 2049  NE2 HIS A 287     6.882  55.515  -2.612  1.00 25.04  A N
ATOM 2050  C   HIS A 287     4.338  57.982   0.748  1.00 33.79  A C
ATOM 2051  O   HIS A 287     3.172  58.276   1.005  1.00 35.09  A O
ATOM 2052  N   PRO A 288     5.106  58.765  -0.023  1.00 33.24  A N
ATOM 2053  CD  PRO A 288     6.543  58.619  -0.309  1.00 32.00  A C
ATOM 2054  CA  PRO A 288     4.585  60.005  -0.599  1.00 33.56  A C
ATOM 2055  CB  PRO A 288     5.720  60.473  -1.502  1.00 32.33  A C
ATOM 2056  CG  PRO A 288     6.925  60.013  -0.759  1.00 32.97  A C
ATOM 2057  C   PRO A 288     3.292  59.834  -1.365  1.00 34.21  A C
ATOM 2058  O   PRO A 288     2.406  60.668  -1.261  1.00 34.89  A O
ATOM 2059  N   TRP A 289     3.181  58.755  -2.132  1.00 35.31  A N
ATOM 2060  CA  TRP A 289     1.976  58.512  -2.931  1.00 35.13  A C
ATOM 2061  CB  TRP A 289     2.175  57.305  -3.856  1.00 33.08  A C
ATOM 2062  CG  TRP A 289     1.049  57.126  -4.821  1.00 32.33  A C
ATOM 2063  CD2 TRP A 289    -0.029  56.181  -4.724  1.00 31.80  A C
ATOM 2064  CE2 TRP A 289    -0.865  56.391  -5.842  1.00 32.43  A C
ATOM 2065  CE3 TRP A 289    -0.367  55.180  -3.801  1.00 31.76  A C
ATOM 2066  CD1 TRP A 289     0.826  57.847  -5.955  1.00 30.36  A C
ATOM 2067  NE1 TRP A 289    -0.319  57.411  -6.573  1.00 32.75  A N
ATOM 2068  CZ2 TRP A 289    -2.025  55.633  -6.065  1.00 32.15  A C
ATOM 2069  CZ3 TRP A 289    -1.521  54.424  -4.022  1.00 30.78  A C
ATOM 2070  CH2 TRP A 289    -2.334  54.657  -5.147  1.00 31.98  A C
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FIGURE 1A-38

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ATOM 2071  C   TRP A 289     0.730  58.273  -2.090  1.00 35.77  A C
ATOM 2072  O   TRP A 289    -0.390  58.469  -2.564  1.00 34.98  A O
ATOM 2073  N   MET A 290     0.930  57.848  -0.846  1.00 37.42  A N
ATOM 2074  CA  MET A 290    -0.176  57.553   0.061  1.00 40.50  A C
ATOM 2075  CB  MET A 290     0.244  56.451   1.037  1.00 38.83  A C
ATOM 2076  CG  MET A 290     0.396  55.060   0.412  1.00 41.30  A C
ATOM 2077  SD  MET A 290    -1.187  54.258   0.044  1.00 43.91  A S
ATOM 2078  CE  MET A 290    -1.484  53.466   1.545  1.00 45.70  A C
ATOM 2079  C   MET A 290    -0.742  58.730   0.865  1.00 41.96  A C
ATOM 2080  O   MET A 290    -1.656  58.541   1.670  1.00 42.54  A O
ATOM 2081  N   GLN A 291    -0.220  59.937   0.657  1.00 43.44  A N
ATOM 2082  CA  GLN A 291    -0.708  61.096   1.416  1.00 45.49  A C
ATOM 2083  CB  GLN A 291     0.405  62.140   1.539  1.00 45.69  A C
ATOM 2084  CG  GLN A 291     1.704  61.575   2.120  1.00 50.80  A C
ATOM 2085  CD  GLN A 291     1.488  60.699   3.371  1.00 53.61  A C
ATOM 2086  OE1 GLN A 291     1.037  61.178   4.419  1.00 54.52  A O
ATOM 2087  NE2 GLN A 291     1.813  59.409   3.254  1.00 51.81  A N
ATOM 2088  C   GLN A 291    -1.983  61.746   0.856  1.00 45.37  A C
ATOM 2089  O   GLN A 291    -2.274  61.648  -0.340  1.00 44.98  A O
ATOM 2090  N   ASP A 292    -2.748  62.393   1.734  1.00 44.99  A N
ATOM 2091  CA  ASP A 292    -3.989  63.065   1.337  1.00 46.00  A C
ATOM 2092  CB  ASP A 292    -3.706  64.114   0.255  1.00 48.62  A C
ATOM 2093  CG  ASP A 292    -2.675  65.131   0.685  1.00 52.60  A C
ATOM 2094  OD1 ASP A 292    -2.888  65.780   1.730  1.00 55.79  A O
ATOM 2095  OD2 ASP A 292    -1.654  65.285  -0.023  1.00 54.82  A O
ATOM 2096  C   ASP A 292    -5.065  62.110   0.816  1.00 44.29  A C
ATOM 2097  O   ASP A 292    -5.781  62.430  -0.127  1.00 43.49  A O
ATOM 2098  N   VAL A 293    -5.180  60.941   1.428  1.00 42.87  A N
ATOM 2099  CA  VAL A 293    -6.179  59.971   1.003  1.00 42.69  A C
ATOM 2100  CB  VAL A 293    -6.008  58.648   1.757  1.00 42.44  A C
ATOM 2101  CG1 VAL A 293    -6.099  58.897   3.258  1.00 43.10  A C
ATOM 2102  CG2 VAL A 293    -7.077  57.666   1.326  1.00 44.50  A C
ATOM 2103  C   VAL A 293    -7.581  60.500   1.287  1.00 42.56  A C
ATOM 2104  O   VAL A 293    -7.812  61.135   2.310  1.00 42.96  A O
ATOM 2105  N   LEU A 294    -8.515  60.240   0.384  1.00 42.46  A N
ATOM 2106  CA  LEU A 294    -9.888  60.691   0.575  1.00 43.08  A C
ATOM 2107  CB  LEU A 294   -10.699  60.558  -0.716  1.00 41.63  A C
ATOM 2108  CG  LEU A 294   -10.348  61.443  -1.902  1.00 42.01  A C
ATOM 2109  CD1 LEU A 294   -11.255  61.096  -3.077  1.00 43.39  A C
ATOM 2110  CD2 LEU A 294   -10.513  62.896  -1.512  1.00 40.37  A C
ATOM 2111  C   LEU A 294   -10.554  59.832   1.625  1.00 44.00  A C
ATOM 2112  O   LEU A 294   -10.097  58.731   1.908  1.00 44.04  A O
ATOM 2113  N   LEU A 295   -11.635  60.344   2.201  1.00 45.58  A N
ATOM 2114  CA  LEU A 295   -12.398  59.596   3.186  1.00 46.90  A C
ATOM 2115  CB  LEU A 295   -13.216  60.537   4.068  1.00 49.61  A C
ATOM 2116  CG  LEU A 295   -12.475  61.125   5.268  1.00 53.00  A C
ATOM 2117  CD1 LEU A 295   -11.200  61.818   4.809  1.00 55.31  A C
ATOM 2118  CD2 LEU A 295   -13.394  62.099   5.991  1.00 54.46  A C
ATOM 2119  C   LEU A 295   -13.333  58.677   2.412  1.00 45.89  A C
ATOM 2120  O   LEU A 295   -13.627  58.918   1.248  1.00 44.99  A O
ATOM 2121  N   PRO A 296   -13.803  57.602   3.047  1.00 46.28  A N
ATOM 2122  CD  PRO A 296   -13.426  57.088   4.377  1.00 45.84  A C
ATOM 2123  CA  PRO A 296   -14.705  56.676   2.357  1.00 46.82  A C
ATOM 2124  CB  PRO A 296   -15.118  55.722   3.468  1.00 46.68  A C
ATOM 2125  CG  PRO A 296   -13.854  55.638   4.294  1.00 46.30  A C
ATOM 2126  C   PRO A 296   -15.901  57.330   1.662  1.00 48.34  A C
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FIGURE 1A-39

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ATOM 2127  O   PRO A 296  -16.122  57.111   0.468  1.00 47.03  A O
ATOM 2128  N   GLN A 297  -16.665  58.134   2.401  1.00 50.55  A N
ATOM 2129  CA  GLN A 297  -17.845  58.792   1.831  1.00 52.11  A C
ATOM 2130  CB  GLN A 297  -18.599  59.585   2.906  1.00 55.20  A C
ATOM 2131  CG  GLN A 297  -20.063  59.878   2.551  1.00 59.51  A C
ATOM 2132  CD  GLN A 297  -20.912  58.611   2.428  1.00 62.56  A C
ATOM 2133  OE1 GLN A 297  -21.025  57.830   3.376  1.00 64.01  A O
ATOM 2134  NE2 GLN A 297  -21.512  58.407   1.257  1.00 63.73  A N
ATOM 2135  C   GLN A 297  -17.472  59.709   0.669  1.00 50.84  A C
ATOM 2136  O   GLN A 297  -18.130  59.693  -0.369  1.00 51.76  A O
ATOM 2137  N   GLU A 298  -16.421  60.504   0.846  1.00 49.24  A N
ATOM 2138  CA  GLU A 298  -15.944  61.400  -0.206  1.00 48.85  A C
ATOM 2139  CB  GLU A 298  -14.665  62.120   0.233  1.00 50.08  A C
ATOM 2140  CG  GLU A 298  -14.870  63.228   1.243  1.00 53.68  A C
ATOM 2141  CD  GLU A 298  -13.576  63.916   1.641  1.00 56.15  A C
ATOM 2142  OE1 GLU A 298  -13.648  65.078   2.097  1.00 59.06  A O
ATOM 2143  OE2 GLU A 298  -12.491  63.302   1.517  1.00 55.91  A O
ATOM 2144  C   GLU A 298  -15.634  60.576  -1.449  1.00 48.61  A C
ATOM 2145  O   GLU A 298  -15.914  60.991  -2.574  1.00 50.16  A O
ATOM 2146  N   THR A 299  -15.046  59.404  -1.232  1.00 46.95  A N
ATOM 2147  CA  THR A 299  -14.689  58.515  -2.323  1.00 45.43  A C
ATOM 2148  CB  THR A 299  -13.978  57.242  -1.799  1.00 44.41  A C
ATOM 2149  OG1 THR A 299  -12.806  57.616  -1.063  1.00 44.50  A O
ATOM 2150  CG2 THR A 299  -13.576  56.337  -2.951  1.00 41.18  A C
ATOM 2151  C   THR A 299  -15.956  58.116  -3.060  1.00 45.01  A C
ATOM 2152  O   THR A 299  -15.998  58.114  -4.288  1.00 43.48  A O
ATOM 2153  N   ALA A 300  -16.995  57.789  -2.299  1.00 45.52  A N
ATOM 2154  CA  ALA A 300  -18.265  57.379  -2.885  1.00 47.38  A C
ATOM 2155  CB  ALA A 300  -19.207  56.917  -1.798  1.00 47.69  A C
ATOM 2156  C   ALA A 300  -18.931  58.476  -3.714  1.00 49.07  A C
ATOM 2157  O   ALA A 300  -19.393  58.216  -4.821  1.00 48.90  A O
ATOM 2158  N   GLU A 301  -18.979  59.700  -3.196  1.00 49.46  A N
ATOM 2159  CA  GLU A 301  -19.628  60.767  -3.949  1.00 51.35  A C
ATOM 2160  CB  GLU A 301  -19.850  62.014  -3.086  1.00 52.64  A C
ATOM 2161  CG  GLU A 301  -19.526  61.837  -1.625  1.00 58.23  A C
ATOM 2162  CD  GLU A 301  -20.355  62.735  -0.728  1.00 60.33  A C
ATOM 2163  OE1 GLU A 301  -21.533  62.393  -0.468  1.00 61.44  A O
ATOM 2164  OE2 GLU A 301  -19.828  63.783  -0.289  1.00 61.57  A O
ATOM 2165  C   GLU A 301  -18.871  61.154  -5.205  1.00 50.37  A C
ATOM 2166  O   GLU A 301  -19.480  61.364  -6.257  1.00 50.57  A O
ATOM 2167  N   ILE A 302  -17.549  61.238  -5.105  1.00 49.01  A N
ATOM 2168  CA  ILE A 302  -16.740  61.618  -6.256  1.00 46.50  A C
ATOM 2169  CB  ILE A 302  -15.304  61.983  -5.843  1.00 46.05  A C
ATOM 2170  CG2 ILE A 302  -14.539  62.526  -7.041  1.00 44.65  A C
ATOM 2171  CG1 ILE A 302  -15.324  63.033  -4.739  1.00 45.36  A C
ATOM 2172  CD1 ILE A 302  -13.946  63.396  -4.228  1.00 43.12  A C
ATOM 2173  C   ILE A 302  -16.642  60.526  -7.317  1.00 46.77  A C
ATOM 2174  O   ILE A 302  -16.766  60.803  -8.509  1.00 46.44  A O
ATOM 2175  N   HIS A 303  -16.449  59.282  -6.879  1.00 47.32  A N
ATOM 2176  CA  HIS A 303  -16.258  58.161  -7.798  1.00 46.13  A C
ATOM 2177  CB  HIS A 303  -14.915  57.490  -7.503  1.00 43.92  A C
ATOM 2178  CG  HIS A 303  -13.735  58.400  -7.637  1.00 40.96  A C
ATOM 2179  CD2 HIS A 303  -12.990  59.034  -6.702  1.00 39.46  A C
ATOM 2180  ND1 HIS A 303  -13.211  58.764  -8.858  1.00 40.55  A N
ATOM 2181  CE1 HIS A 303  -12.192  59.585  -8.669  1.00 40.10  A C
ATOM 2182  NE2 HIS A 303  -12.037  59.765  -7.369  1.00 38.16  A N
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FIGURE 1A-40

```
ATOM 2183  C   HIS A 303  -17.298  57.059  -7.869  1.00 47.55  A C
ATOM 2184  O   HIS A 303  -17.369  56.362  -8.871  1.00 46.87  A O
ATOM 2185  N   LEU A 304  -18.102  56.879  -6.832  1.00 50.27  A N
ATOM 2186  CA  LEU A 304  -19.055  55.782  -6.871  1.00 53.75  A C
ATOM 2187  CB  LEU A 304  -18.945  54.974  -5.581  1.00 52.58  A C
ATOM 2188  CG  LEU A 304  -17.532  54.498  -5.247  1.00 52.64  A C
ATOM 2189  CD1 LEU A 304  -17.553  53.725  -3.938  1.00 51.38  A C
ATOM 2190  CD2 LEU A 304  -17.000  53.633  -6.377  1.00 50.53  A C
ATOM 2191  C   LEU A 304  -20.512  56.133  -7.140  1.00 57.27  A C
ATOM 2192  O   LEU A 304  -21.220  55.361  -7.795  1.00 58.13  A O
ATOM 2193  N   HIS A 305  -20.967  57.277  -6.639  1.00 59.77  A N
ATOM 2194  CA  HIS A 305  -22.356  57.678  -6.854  1.00 62.72  A C
ATOM 2195  CB  HIS A 305  -22.753  58.824  -5.908  1.00 63.91  A C
ATOM 2196  CG  HIS A 305  -22.703  58.460  -4.452  1.00 65.66  A C
ATOM 2197  CD2 HIS A 305  -22.583  59.232  -3.344  1.00 65.80  A C
ATOM 2198  ND1 HIS A 305  -22.820  57.161  -4.001  1.00 66.63  A N
ATOM 2199  CE1 HIS A 305  -22.773  57.149  -2.679  1.00 65.63  A C
ATOM 2200  NE2 HIS A 305  -22.630  58.392  -2.256  1.00 65.61  A N
ATOM 2201  C   HIS A 305  -22.579  58.101  -8.307  1.00 63.21  A C
ATOM 2202  O   HIS A 305  -23.418  57.462  -8.984  1.00 62.66  A O
ATOM 2203  OXT HIS A 305  -21.906  59.059  -8.751  1.00 64.32  A O
TER        1   HIS A 305                                      A
HET  2204  O   HOH W   1    4.729  45.185   8.432  1.00 36.65  W O
HET  2205  O   HOH W   2    8.337  38.878   6.694  1.00 29.30  W O
HET  2206  O   HOH W   3  -15.034  38.244   5.973  1.00 30.95  W O
HET  2207  O   HOH W   4   -2.862  39.196   5.414  1.00 32.31  W O
HET  2208  O   HOH W   5    6.054  34.433   9.050  1.00 33.57  W O
HET  2209  O   HOH W   6    3.237  37.372  -8.066  1.00 30.25  W O
HET  2210  O   HOH W   7   -7.881  33.380   2.673  1.00 38.15  W O
HET  2211  O   HOH W   8  -17.583  44.864   8.863  1.00 44.55  W O
HET  2212  O   HOH W   9    0.775  39.030 -11.265  1.00 36.93  W O
HET  2213  O   HOH W  10    9.335  40.074 -14.685  1.00 43.50  W O
HET  2214  O   HOH W  11  -19.621  41.536  -7.696  1.00 33.51  W O
HET  2215  O   HOH W  12  -11.064  26.602   6.568  1.00 43.48  W O
HET  2216  O   HOH W  13  -14.208  33.995   5.025  1.00 30.27  W O
HET  2217  O   HOH W  14    5.736  37.612   9.167  1.00 48.52  W O
HET  2218  O   HOH W  15  -10.471  53.328 -17.070  1.00 48.31  W O
HET  2219  O   HOH W  16  -11.358  55.717 -12.222  1.00 43.92  W O
HET  2220  O   HOH W  17  -16.003  33.941   0.645  1.00 45.72  W O
HET  2221  O   HOH W  18   -8.614  42.805 -12.192  1.00 53.74  W O
HET  2222  O   HOH W  19   -3.431  54.815  10.359  1.00 29.09  W O
HET  2223  O   HOH W  20    4.243  48.144   9.917  1.00 37.03  W O
HET  2224  O   HOH W  21  -15.795  36.095   4.235  1.00 32.05  W O
HET  2225  O   HOH W  22    1.775  48.883  10.671  1.00 36.50  W O
HET  2226  O   HOH W  23   -2.046  38.097   0.599  1.00 36.51  W O
HET  2227  O   HOH W  24   -7.600  59.349  -2.247  1.00 40.11  W O
HET  2228  O   HOH W  25   15.256  42.922  -3.737  1.00 34.53  W O
HET  2229  O   HOH W  26   -4.869  59.163 -12.225  1.00 48.39  W O
HET  2230  O   HOH W  27  -12.953  49.826   4.770  1.00 40.74  W O
HET  2231  O   HOH W  28  -10.464  49.746   6.029  1.00 32.90  W O
HET  2232  O   HOH W  29  -10.506  56.045   2.224  1.00 39.16  W O
HET  2233  O   HOH W  30    8.105  55.304   3.245  1.00 42.00  W O
HET  2234  O   HOH W  31   -4.327  54.719 -13.591  1.00 46.02  W O
HET  2235  O   HOH W  32   -6.059  62.619   4.254  1.00 62.75  W O
HET  2236  O   HOH W  33   -2.736  59.731   3.907  1.00 46.12  W O
HET  2237  O   HOH W  34   -6.764  39.019 -10.922  1.00 53.57  W O
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FIGURE 1A-41

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HET  2238  O    HOH W  35  -25.044  22.956   4.085  1.00 44.71  W O
HET  2239  O    HOH W  36   14.715  38.285   2.631  1.00 55.84  W O
HET  2240  O    HOH W  37   11.001  46.043  -8.013  1.00 42.10  W O
HET  2241  O    HOH W  38    3.450  26.324   7.066  1.00 53.95  W O
HET  2242  O    HOH W  39   -9.091  46.586 -16.814  1.00 56.14  W O
HET  2243  O    HOH W  40   -4.024  36.587  -4.048  1.00 54.77  W O
HET  2244  O    HOH W  41  -11.752  41.569  15.549  1.00 66.78  W O
HET  2245  O    HOH W  42   -8.812  52.840   9.523  1.00 39.92  W O
HET  2246  O    HOH W  43    5.247  25.652  -6.395  1.00 59.41  W O
HET  2247  O    HOH W  44    8.208  50.015  10.135  1.00 43.70  W O
HET  2248  O    HOH W  45  -12.430  33.563  -2.836  1.00 49.91  W O
HET  2249  O    HOH W  46   15.754  39.773 -12.048  1.00 51.85  W O
HET  2250  O    HOH W  48    9.576  24.077   1.510  1.00 48.03  W O
HET  2251  O    HOH W  49  -29.791  30.650  -7.362  1.00 41.79  W O
HET  2252  O    HOH W  50   -8.219  50.900 -18.374  1.00 54.04  W O
HET  2253  O    HOH W  51  -31.835  29.438  -3.076  1.00 46.44  W O
HET  2254  O    HOH W  52   -0.291  35.831  -0.130  1.00 49.24  W O
HET  2255  O    HOH W  53  -23.920  50.333   5.123  1.00 69.84  W O
HET  2256  O    HOH W  54   -8.705  25.244   4.369  1.00 70.95  W O
HET  2257  O    HOH W  55    7.699  65.340 -13.336  1.00 73.43  W O
HET  2258  O    HOH W  56  -18.668  17.137   3.217  1.00 71.39  W O
HET  2259  O    HOH W  57   -5.891  27.604   4.689  1.00 44.14  W O
HET  2260  O    HOH W  58    3.976  63.972  -3.122  1.00 59.85  W O
HET  2261  O    HOH W  59  -24.721  56.614   9.542  1.00 73.38  W O
HET  2262  O    HOH W  60   -6.171  61.666  -2.733  1.00 36.34  W O
HET  2263  O    HOH W  61   -2.392  34.230  15.975  1.00 52.99  W O
HET  2264  O    HOH W  62  -16.013  18.503  13.049  1.00 62.20  W O
HET  2265  O    HOH W  63   11.124  43.448  -8.738  1.00 32.24  W O
HET  2266  O    HOH W  64   -1.732  38.022   3.562  1.00 33.45  W O
HET  2267  O    HOH W  65    8.642  36.390   2.403  1.00 41.53  W O
HET  2268  O    HOH W  66   -7.050  26.613   1.351  1.00 61.53  W O
HET  2269  O    HOH W  67   -7.171  63.951  -4.127  1.00 50.66  W O
HET  2270  O    HOH W  68  -17.323  35.775   2.290  1.00 59.03  W O
HET  2271  O    HOH W  69    1.399  37.061  -1.834  1.00 58.10  W O
HET  2272  O    HOH W  70    1.126  61.747 -12.741  1.00 46.10  W O
HET  2273  O    HOH W  71  -17.674  25.405  -4.968  1.00 51.21  W O
HET  2274  O    HOH W  72  -19.485  24.431  -2.758  1.00 48.93  W O
HET  2275  O    HOH W  73  -24.283  50.294   0.323  1.00 84.16  W O
HET  2276  O    HOH W  74   -1.055  62.318  -3.009  1.00 47.94  W O
HET  2277  O    HOH W  75    2.981  45.368  10.620  1.00 69.95  W O
HET  2278  O    HOH W  76    9.636  62.038 -15.040  1.00 46.37  W O
HET  2279  O    HOH W  77  -13.384  57.328 -11.070  1.00 37.08  W O
HET  2280  O    HOH W  78   10.237  53.331  -9.999  1.00 61.83  W O
HET  2281  O    HOH W  79    7.191  43.535   4.588  1.00 38.92  W O
HET  2282  O    HOH W  80  -15.831  58.660   5.321  1.00 51.03  W O
HET  2283  O    HOH W  81  -18.532  37.417  -8.010  1.00 89.56  W O
HET  2284  O    HOH W  82  -14.112  35.296  -3.400  1.00 49.35  W O
HET  2285  O5'  ADE Z   1  -16.339  36.219  -4.866  1.00 92.13  Z O
HET  2286  C5'  ADE Z   1  -17.619  35.660  -4.722  1.00 91.01  Z C
HET  2287  C4'  ADE Z   1  -18.711  36.734  -4.721  1.00 90.47  Z C
HET  2288  O4'  ADE Z   1  -19.703  36.424  -3.759  1.00 89.54  Z O
HET  2289  C1'  ADE Z   1  -20.212  37.595  -3.129  1.00 88.81  Z C
HET  2290  C2'  ADE Z   1  -19.483  38.766  -3.796  1.00 90.11  Z C
HET  2291  C3'  ADE Z   1  -18.223  38.128  -4.344  1.00 90.49  Z C
HET  2292  O3'  ADE Z   1  -17.746  38.829  -5.506  1.00 91.87  Z O
HET  2293  N9   ADE Z   1  -19.913  37.547  -1.682  1.00 86.36  Z N
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FIGURE 1A-42

```
HET   2294  C4   ADE Z   1  -20.494  38.379  -0.732  1.00 85.38   Z C
HET   2295  N3   ADE Z   1  -21.418  39.353  -0.867  1.00 84.24   Z N
HET   2296  C2   ADE Z   1  -21.794  39.981   0.251  1.00 84.14   Z C
HET   2297  N1   ADE Z   1  -21.320  39.711   1.479  1.00 83.50   Z N
HET   2298  C6   ADE Z   1  -20.401  38.741   1.595  1.00 83.78   Z C
HET   2299  N6   ADE Z   1  -19.937  38.487   2.830  1.00 84.36   Z N
HET   2300  C5   ADE Z   1  -19.949  38.036   0.520  1.00 84.41   Z C
HET   2301  N7   ADE Z   1  -19.039  37.003   0.337  1.00 84.56   Z N
HET   2302  C8   ADE Z   1  -19.064  36.756  -0.990  1.00 85.21   Z C
HET   2303  O2'  ADE Z   1  -20.235  39.239  -4.880  1.00 90.38   Z O
END
```

FIGURE 2A-1

ATOM	Type	Resid	#	X	Y	Z	Occ	B	
ATOM	1	CB	PRO A	33	-33.439	25.955	13.809	1.00	68.92	A C
ATOM	2	CG	PRO A	33	-33.315	26.836	15.047	1.00	68.97	A C
ATOM	3	C	PRO A	33	-31.734	27.170	12.421	1.00	68.56	A C
ATOM	4	O	PRO A	33	-32.381	28.222	12.521	1.00	68.72	A O
ATOM	5	N	PRO A	33	-31.146	26.095	14.528	1.00	68.98	A N
ATOM	6	CD	PRO A	33	-31.966	26.480	15.691	1.00	69.03	A C
ATOM	7	CA	PRO A	33	-32.004	25.970	13.323	1.00	68.82	A C
ATOM	8	N	LEU A	34	-30.721	27.000	11.578	1.00	68.12	A N
ATOM	9	CA	LEU A	34	-30.288	28.011	10.620	1.00	67.49	A C
ATOM	10	CB	LEU A	34	-28.977	27.545	9.988	1.00	67.61	A C
ATOM	11	CG	LEU A	34	-28.851	27.574	8.469	1.00	67.72	A C
ATOM	12	CD1	LEU A	34	-28.538	28.979	7.986	1.00	67.76	A C
ATOM	13	CD2	LEU A	34	-27.760	26.625	8.045	1.00	67.71	A C
ATOM	14	C	LEU A	34	-31.353	28.226	9.541	1.00	66.97	A C
ATOM	15	O	LEU A	34	-31.439	29.290	8.926	1.00	66.98	A O
ATOM	16	N	GLU A	35	-32.175	27.207	9.339	1.00	66.24	A N
ATOM	17	CA	GLU A	35	-33.220	27.244	8.333	1.00	65.51	A C
ATOM	18	CB	GLU A	35	-33.728	25.817	8.083	1.00	65.93	A C
ATOM	19	CG	GLU A	35	-33.029	24.719	8.887	1.00	66.52	A C
ATOM	20	CD	GLU A	35	-32.191	23.822	8.001	1.00	66.93	A C
ATOM	21	OE1	GLU A	35	-32.634	23.543	6.870	1.00	67.42	A O
ATOM	22	OE2	GLU A	35	-31.116	23.361	8.435	1.00	67.11	A O
ATOM	23	C	GLU A	35	-34.380	28.141	8.746	1.00	64.68	A C
ATOM	24	O	GLU A	35	-35.136	28.641	7.901	1.00	64.75	A O
ATOM	25	N	SER A	36	-34.530	28.335	10.050	1.00	63.45	A N
ATOM	26	CA	SER A	36	-35.620	29.150	10.573	1.00	62.08	A C
ATOM	27	CB	SER A	36	-36.034	28.606	11.953	1.00	62.37	A C
ATOM	28	OG	SER A	36	-36.762	29.576	12.702	1.00	62.40	A O
ATOM	29	C	SER A	36	-35.310	30.645	10.683	1.00	60.89	A C
ATOM	30	O	SER A	36	-36.130	31.499	10.335	1.00	60.77	A O
ATOM	31	N	GLN A	37	-34.109	30.956	11.150	1.00	59.40	A N
ATOM	32	CA	GLN A	37	-33.743	32.348	11.350	1.00	57.86	A C
ATOM	33	CB	GLN A	37	-32.798	32.462	12.546	1.00	58.03	A C
ATOM	34	CG	GLN A	37	-31.761	31.371	12.597	1.00	58.32	A C
ATOM	35	CD	GLN A	37	-31.032	31.353	13.918	1.00	58.47	A C
ATOM	36	OE1	GLN A	37	-30.785	32.414	14.498	1.00	58.28	A O
ATOM	37	NE2	GLN A	37	-30.661	30.157	14.396	1.00	58.51	A N
ATOM	38	C	GLN A	37	-33.167	33.118	10.161	1.00	56.54	A C
ATOM	39	O	GLN A	37	-32.866	34.296	10.281	1.00	56.47	A O
ATOM	40	N	TYR A	38	-32.995	32.468	9.020	1.00	54.98	A N
ATOM	41	CA	TYR A	38	-32.456	33.143	7.837	1.00	53.50	A C
ATOM	42	CB	TYR A	38	-30.997	32.740	7.613	1.00	52.98	A C
ATOM	43	CG	TYR A	38	-30.069	33.229	8.697	1.00	52.22	A C
ATOM	44	CD1	TYR A	38	-29.668	34.561	8.753	1.00	51.93	A C
ATOM	45	CE1	TYR A	38	-28.889	35.028	9.804	1.00	51.81	A C
ATOM	46	CD2	TYR A	38	-29.661	32.377	9.715	1.00	51.99	A C
ATOM	47	CE2	TYR A	38	-28.888	32.830	10.763	1.00	51.86	A C
ATOM	48	CZ	TYR A	38	-28.507	34.154	10.805	1.00	51.71	A C
ATOM	49	OH	TYR A	38	-27.749	34.603	11.856	1.00	51.56	A O
ATOM	50	C	TYR A	38	-33.254	32.797	6.595	1.00	52.72	A C
ATOM	51	O	TYR A	38	-33.608	31.637	6.363	1.00	52.69	A O
ATOM	52	N	GLN A	39	-33.543	33.811	5.794	1.00	51.74	A N
ATOM	53	CA	GLN A	39	-34.261	33.585	4.555	1.00	50.71	A C
ATOM	54	CB	GLN A	39	-35.319	34.656	4.333	1.00	51.43	A C

FIGURE 2A-2

```
ATOM    55  CG  GLN A  39   -36.030  34.527   2.999  1.00 52.66  A C
ATOM    56  CD  GLN A  39   -37.264  35.401   2.909  1.00 53.46  A C
ATOM    57  OE1 GLN A  39   -37.255  36.560   3.332  1.00 53.97  A O
ATOM    58  NE2 GLN A  39   -38.334  34.855   2.339  1.00 53.96  A N
ATOM    59  C   GLN A  39   -33.234  33.620   3.430  1.00 49.42  A C
ATOM    60  O   GLN A  39   -32.733  34.675   3.062  1.00 49.37  A O
ATOM    61  N   VAL A  40   -32.926  32.446   2.894  1.00 47.91  A N
ATOM    62  CA  VAL A  40   -31.945  32.314   1.832  1.00 46.36  A C
ATOM    63  CB  VAL A  40   -31.645  30.833   1.543  1.00 46.34  A C
ATOM    64  CG1 VAL A  40   -30.395  30.720   0.680  1.00 46.31  A C
ATOM    65  CG2 VAL A  40   -31.481  30.096   2.856  1.00 46.19  A C
ATOM    66  C   VAL A  40   -32.370  32.998   0.538  1.00 45.26  A C
ATOM    67  O   VAL A  40   -33.548  33.015   0.197  1.00 45.28  A O
ATOM    68  N   GLY A  41   -31.395  33.580  -0.163  1.00 43.81  A N
ATOM    69  CA  GLY A  41   -31.644  34.243  -1.436  1.00 41.79  A C
ATOM    70  C   GLY A  41   -30.846  33.595  -2.559  1.00 40.51  A C
ATOM    71  O   GLY A  41   -30.505  32.418  -2.478  1.00 40.47  A O
ATOM    72  N   PRO A  42   -30.522  34.334  -3.625  1.00 39.41  A N
ATOM    73  CD  PRO A  42   -30.857  35.734  -3.931  1.00 39.12  A C
ATOM    74  CA  PRO A  42   -29.757  33.728  -4.718  1.00 38.62  A C
ATOM    75  CB  PRO A  42   -29.892  34.758  -5.836  1.00 38.61  A C
ATOM    76  CG  PRO A  42   -29.923  36.038  -5.090  1.00 38.85  A C
ATOM    77  C   PRO A  42   -28.295  33.421  -4.395  1.00 37.83  A C
ATOM    78  O   PRO A  42   -27.740  33.943  -3.432  1.00 37.64  A O
ATOM    79  N   LEU A  43   -27.679  32.580  -5.223  1.00 36.89  A N
ATOM    80  CA  LEU A  43   -26.279  32.212  -5.056  1.00 36.00  A C
ATOM    81  CB  LEU A  43   -25.952  30.986  -5.921  1.00 35.82  A C
ATOM    82  CG  LEU A  43   -24.510  30.459  -5.937  1.00 35.60  A C
ATOM    83  CD1 LEU A  43   -24.213  29.726  -4.628  1.00 35.30  A C
ATOM    84  CD2 LEU A  43   -24.320  29.507  -7.118  1.00 35.38  A C
ATOM    85  C   LEU A  43   -25.391  33.380  -5.485  1.00 35.42  A C
ATOM    86  O   LEU A  43   -25.494  33.855  -6.615  1.00 35.43  A O
ATOM    87  N   LEU A  44   -24.527  33.849  -4.590  1.00 34.64  A N
ATOM    88  CA  LEU A  44   -23.618  34.940  -4.930  1.00 33.82  A C
ATOM    89  CB  LEU A  44   -23.145  35.663  -3.666  1.00 33.55  A C
ATOM    90  CG  LEU A  44   -24.244  36.441  -2.935  1.00 33.61  A C
ATOM    91  CD1 LEU A  44   -23.702  37.021  -1.636  1.00 32.90  A C
ATOM    92  CD2 LEU A  44   -24.776  37.552  -3.846  1.00 33.31  A C
ATOM    93  C   LEU A  44   -22.416  34.398  -5.704  1.00 33.40  A C
ATOM    94  O   LEU A  44   -21.790  35.122  -6.467  1.00 33.46  A O
ATOM    95  N   GLY A  45   -22.100  33.119  -5.510  1.00 32.91  A N
ATOM    96  CA  GLY A  45   -20.984  32.512  -6.221  1.00 31.85  A C
ATOM    97  C   GLY A  45   -20.533  31.251  -5.523  1.00 31.40  A C
ATOM    98  O   GLY A  45   -20.986  30.963  -4.416  1.00 31.33  A O
ATOM    99  N   SER A  46   -19.663  30.484  -6.160  1.00 30.95  A N
ATOM   100  CA  SER A  46   -19.149  29.270  -5.541  1.00 31.12  A C
ATOM   101  CB  SER A  46   -20.060  28.069  -5.818  1.00 31.08  A C
ATOM   102  OG  SER A  46   -19.862  27.571  -7.133  1.00 30.98  A O
ATOM   103  C   SER A  46   -17.770  28.995  -6.101  1.00 31.17  A C
ATOM   104  O   SER A  46   -17.409  29.512  -7.161  1.00 31.22  A O
ATOM   105  N   GLY A  47   -16.997  28.182  -5.393  1.00 31.38  A N
ATOM   106  CA  GLY A  47   -15.659  27.860  -5.856  1.00 31.42  A C
ATOM   107  C   GLY A  47   -14.839  27.186  -4.778  1.00 31.58  A C
ATOM   108  O   GLY A  47   -15.379  26.403  -3.989  1.00 31.44  A O
ATOM   109  N   GLY A  48   -13.543  27.503  -4.731  1.00 31.56  A N
ATOM   110  CA  GLY A  48   -12.656  26.909  -3.740  1.00 31.63  A C
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FIGURE 2A-3

```
ATOM  111  C   GLY A  48  -13.153  27.090  -2.322  1.00 31.67  A C
ATOM  112  O   GLY A  48  -12.999  26.214  -1.483  1.00 31.97  A O
ATOM  113  N   PHE A  49  -13.765  28.236  -2.063  1.00 31.50  A N
ATOM  114  CA  PHE A  49  -14.303  28.573  -0.749  1.00 31.43  A C
ATOM  115  CB  PHE A  49  -14.489  30.090  -0.680  1.00 31.47  A C
ATOM  116  CG  PHE A  49  -15.107  30.659  -1.926  1.00 31.48  A C
ATOM  117  CD1 PHE A  49  -14.300  31.130  -2.963  1.00 31.34  A C
ATOM  118  CD2 PHE A  49  -16.490  30.604  -2.116  1.00 31.40  A C
ATOM  119  CE1 PHE A  49  -14.861  31.531  -4.186  1.00 31.27  A C
ATOM  120  CE2 PHE A  49  -17.066  30.998  -3.325  1.00 31.39  A C
ATOM  121  CZ  PHE A  49  -16.249  31.462  -4.368  1.00 31.51  A C
ATOM  122  C   PHE A  49  -15.646  27.898  -0.409  1.00 31.30  A C
ATOM  123  O   PHE A  49  -16.083  27.943   0.735  1.00 31.81  A O
ATOM  124  N   GLY A  50  -16.311  27.293  -1.391  1.00 30.90  A N
ATOM  125  CA  GLY A  50  -17.599  26.659  -1.127  1.00 30.18  A C
ATOM  126  C   GLY A  50  -18.704  27.375  -1.888  1.00 29.87  A C
ATOM  127  O   GLY A  50  -18.472  27.853  -3.000  1.00 30.04  A O
ATOM  128  N   SER A  51  -19.900  27.470  -1.315  1.00 29.34  A N
ATOM  129  CA  SER A  51  -20.999  28.146  -2.004  1.00 29.12  A C
ATOM  130  CB  SER A  51  -22.106  27.146  -2.358  1.00 28.80  A C
ATOM  131  OG  SER A  51  -21.643  26.178  -3.279  1.00 28.08  A O
ATOM  132  C   SER A  51  -21.551  29.250  -1.120  1.00 29.20  A C
ATOM  133  O   SER A  51  -21.849  29.021   0.043  1.00 29.11  A O
ATOM  134  N   VAL A  52  -21.678  30.452  -1.671  1.00 29.54  A N
ATOM  135  CA  VAL A  52  -22.155  31.591  -0.898  1.00 29.85  A C
ATOM  136  CB  VAL A  52  -21.088  32.713  -0.884  1.00 29.80  A C
ATOM  137  CG1 VAL A  52  -21.565  33.903  -0.040  1.00 29.58  A C
ATOM  138  CG2 VAL A  52  -19.784  32.164  -0.338  1.00 29.49  A C
ATOM  139  C   VAL A  52  -23.467  32.151  -1.433  1.00 30.22  A C
ATOM  140  O   VAL A  52  -23.580  32.465  -2.621  1.00 30.11  A O
ATOM  141  N   TYR A  53  -24.446  32.286  -0.539  1.00 30.75  A N
ATOM  142  CA  TYR A  53  -25.766  32.799  -0.894  1.00 31.44  A C
ATOM  143  CB  TYR A  53  -26.880  31.821  -0.503  1.00 30.67  A C
ATOM  144  CG  TYR A  53  -26.828  30.465  -1.154  1.00 30.19  A C
ATOM  145  CD1 TYR A  53  -25.973  29.480  -0.675  1.00 29.90  A C
ATOM  146  CE1 TYR A  53  -25.915  28.236  -1.273  1.00 29.83  A C
ATOM  147  CD2 TYR A  53  -27.631  30.169  -2.257  1.00 29.85  A C
ATOM  148  CE2 TYR A  53  -27.579  28.920  -2.870  1.00 29.73  A C
ATOM  149  CZ  TYR A  53  -26.717  27.962  -2.370  1.00 29.54  A C
ATOM  150  OH  TYR A  53  -26.625  26.733  -2.970  1.00 29.75  A O
ATOM  151  C   TYR A  53  -26.089  34.096  -0.190  1.00 32.49  A C
ATOM  152  O   TYR A  53  -25.651  34.342   0.943  1.00 32.55  A O
ATOM  153  N   SER A  54  -26.896  34.908  -0.860  1.00 33.79  A N
ATOM  154  CA  SER A  54  -27.355  36.156  -0.296  1.00 35.19  A C
ATOM  155  CB  SER A  54  -28.025  37.010  -1.364  1.00 35.34  A C
ATOM  156  OG  SER A  54  -28.544  38.202  -0.801  1.00 36.05  A O
ATOM  157  C   SER A  54  -28.392  35.691   0.714  1.00 36.20  A C
ATOM  158  O   SER A  54  -28.929  34.593   0.585  1.00 36.05  A O
ATOM  159  N   GLY A  55  -28.658  36.510   1.724  1.00 37.36  A N
ATOM  160  CA  GLY A  55  -29.634  36.138   2.728  1.00 38.63  A C
ATOM  161  C   GLY A  55  -30.111  37.324   3.539  1.00 39.79  A C
ATOM  162  O   GLY A  55  -29.612  38.444   3.402  1.00 39.69  A O
ATOM  163  N   ILE A  56  -31.098  37.075   4.386  1.00 40.98  A N
ATOM  164  CA  ILE A  56  -31.648  38.105   5.240  1.00 42.29  A C
ATOM  165  CB  ILE A  56  -32.880  38.754   4.597  1.00 42.65  A C
ATOM  166  CG2 ILE A  56  -32.460  39.669   3.455  1.00 42.38  A C
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FIGURE 2A-4

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ATOM  167  CG1 ILE A  56  -33.807  37.674   4.051  1.00 43.32  A C
ATOM  168  CD1 ILE A  56  -34.942  38.233   3.194  1.00 43.93  A C
ATOM  169  C   ILE A  56  -32.029  37.438   6.546  1.00 42.98  A C
ATOM  170  O   ILE A  56  -32.676  36.397   6.553  1.00 43.15  A O
ATOM  171  N   ARG A  57  -31.592  38.015   7.653  1.00 43.89  A N
ATOM  172  CA  ARG A  57  -31.903  37.445   8.950  1.00 45.13  A C
ATOM  173  CB  ARG A  57  -31.023  38.071  10.029  1.00 45.11  A C
ATOM  174  CG  ARG A  57  -31.164  37.417  11.379  1.00 45.41  A C
ATOM  175  CD  ARG A  57  -30.741  38.377  12.459  1.00 45.80  A C
ATOM  176  NE  ARG A  57  -29.322  38.306  12.776  1.00 46.07  A N
ATOM  177  CZ  ARG A  57  -28.614  39.332  13.233  1.00 46.15  A C
ATOM  178  NH1 ARG A  57  -29.191  40.513  13.417  1.00 46.30  A N
ATOM  179  NH2 ARG A  57  -27.331  39.174  13.514  1.00 46.43  A N
ATOM  180  C   ARG A  57  -33.372  37.734   9.240  1.00 45.85  A C
ATOM  181  O   ARG A  57  -33.755  38.885   9.443  1.00 45.97  A O
ATOM  182  N   VAL A  58  -34.192  36.688   9.241  1.00 46.69  A N
ATOM  183  CA  VAL A  58  -35.623  36.837   9.487  1.00 47.53  A C
ATOM  184  CB  VAL A  58  -36.290  35.473   9.712  1.00 47.64  A C
ATOM  185  CG1 VAL A  58  -37.806  35.642   9.740  1.00 47.75  A C
ATOM  186  CG2 VAL A  58  -35.868  34.504   8.615  1.00 47.80  A C
ATOM  187  C   VAL A  58  -35.891  37.705  10.713  1.00 48.02  A C
ATOM  188  O   VAL A  58  -36.840  38.483  10.746  1.00 48.17  A O
ATOM  189  N   SER A  59  -35.037  37.565  11.718  1.00 48.55  A N
ATOM  190  CA  SER A  59  -35.170  38.325  12.953  1.00 48.90  A C
ATOM  191  CB  SER A  59  -33.950  38.067  13.847  1.00 49.18  A C
ATOM  192  OG  SER A  59  -34.014  38.843  15.029  1.00 49.98  A O
ATOM  193  C   SER A  59  -35.347  39.833  12.747  1.00 48.85  A C
ATOM  194  O   SER A  59  -36.371  40.396  13.132  1.00 48.96  A O
ATOM  195  N   ASP A  60  -34.360  40.488  12.139  1.00 48.60  A N
ATOM  196  CA  ASP A  60  -34.439  41.936  11.936  1.00 48.13  A C
ATOM  197  CB  ASP A  60  -33.460  42.639  12.884  1.00 48.62  A C
ATOM  198  CG  ASP A  60  -32.017  42.207  12.670  1.00 49.10  A C
ATOM  199  OD1 ASP A  60  -31.762  41.000  12.515  1.00 49.38  A O
ATOM  200  OD2 ASP A  60  -31.126  43.079  12.674  1.00 49.88  A O
ATOM  201  C   ASP A  60  -34.193  42.413  10.511  1.00 47.56  A C
ATOM  202  O   ASP A  60  -33.898  43.584  10.295  1.00 47.60  A O
ATOM  203  N   ASN A  61  -34.317  41.509   9.545  1.00 46.70  A N
ATOM  204  CA  ASN A  61  -34.096  41.841   8.139  1.00 45.86  A C
ATOM  205  CB  ASN A  61  -35.055  42.946   7.691  1.00 46.59  A C
ATOM  206  CG  ASN A  61  -36.497  42.514   7.764  1.00 47.48  A C
ATOM  207  OD1 ASN A  61  -36.867  41.453   7.247  1.00 47.82  A O
ATOM  208  ND2 ASN A  61  -37.327  43.329   8.407  1.00 47.61  A N
ATOM  209  C   ASN A  61  -32.663  42.259   7.820  1.00 44.63  A C
ATOM  210  O   ASN A  61  -32.395  42.845   6.768  1.00 44.56  A O
ATOM  211  N   LEU A  62  -31.745  41.962   8.729  1.00 43.14  A N
ATOM  212  CA  LEU A  62  -30.348  42.293   8.508  1.00 41.54  A C
ATOM  213  CB  LEU A  62  -29.511  41.908   9.718  1.00 41.34  A C
ATOM  214  CG  LEU A  62  -28.013  42.167   9.554  1.00 41.11  A C
ATOM  215  CD1 LEU A  62  -27.767  43.667   9.480  1.00 40.46  A C
ATOM  216  CD2 LEU A  62  -27.249  41.552  10.725  1.00 40.72  A C
ATOM  217  C   LEU A  62  -29.862  41.490   7.317  1.00 40.50  A C
ATOM  218  O   LEU A  62  -30.001  40.265   7.295  1.00 40.43  A O
ATOM  219  N   PRO A  63  -29.308  42.164   6.299  1.00 39.40  A N
ATOM  220  CD  PRO A  63  -29.262  43.620   6.081  1.00 39.19  A C
ATOM  221  CA  PRO A  63  -28.811  41.439   5.125  1.00 38.48  A C
ATOM  222  CB  PRO A  63  -28.570  42.547   4.102  1.00 38.60  A C
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FIGURE 2A-5

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ATOM  223  CG  PRO A  63  -28.269  43.740   4.955  1.00 39.02  A C
ATOM  224  C   PRO A  63  -27.543  40.677   5.483  1.00 37.43  A C
ATOM  225  O   PRO A  63  -26.662  41.206   6.159  1.00 37.41  A O
ATOM  226  N   VAL A  64  -27.466  39.425   5.049  1.00 36.31  A N
ATOM  227  CA  VAL A  64  -26.307  38.590   5.336  1.00 35.09  A C
ATOM  228  CB  VAL A  64  -26.625  37.577   6.445  1.00 35.05  A C
ATOM  229  CG1 VAL A  64  -26.970  38.302   7.728  1.00 34.98  A C
ATOM  230  CG2 VAL A  64  -27.772  36.673   6.005  1.00 34.82  A C
ATOM  231  C   VAL A  64  -25.851  37.796   4.117  1.00 34.54  A C
ATOM  232  O   VAL A  64  -26.457  37.868   3.054  1.00 34.17  A O
ATOM  233  N   ALA A  65  -24.765  37.046   4.292  1.00 34.00  A N
ATOM  234  CA  ALA A  65  -24.228  36.180   3.252  1.00 33.60  A C
ATOM  235  CB  ALA A  65  -22.891  36.693   2.735  1.00 33.40  A C
ATOM  236  C   ALA A  65  -24.053  34.854   3.956  1.00 33.40  A C
ATOM  237  O   ALA A  65  -23.492  34.798   5.043  1.00 33.32  A O
ATOM  238  N   ILE A  66  -24.553  33.790   3.342  1.00 33.33  A N
ATOM  239  CA  ILE A  66  -24.481  32.462   3.932  1.00 33.38  A C
ATOM  240  CB  ILE A  66  -25.898  31.831   3.953  1.00 33.21  A C
ATOM  241  CG2 ILE A  66  -25.898  30.534   4.734  1.00 33.04  A C
ATOM  242  CG1 ILE A  66  -26.876  32.825   4.595  1.00 33.16  A C
ATOM  243  CD1 ILE A  66  -28.348  32.397   4.581  1.00 33.04  A C
ATOM  244  C   ILE A  66  -23.486  31.583   3.165  1.00 33.63  A C
ATOM  245  O   ILE A  66  -23.674  31.282   1.985  1.00 33.48  A O
ATOM  246  N   LYS A  67  -22.416  31.184   3.847  1.00 33.92  A N
ATOM  247  CA  LYS A  67  -21.382  30.370   3.228  1.00 34.25  A C
ATOM  248  CB  LYS A  67  -20.002  30.952   3.539  1.00 34.08  A C
ATOM  249  CG  LYS A  67  -18.918  30.383   2.655  1.00 34.44  A C
ATOM  250  CD  LYS A  67  -17.617  31.147   2.810  1.00 34.86  A C
ATOM  251  CE  LYS A  67  -16.739  30.521   3.847  1.00 34.71  A C
ATOM  252  NZ  LYS A  67  -16.095  29.292   3.308  1.00 35.10  A N
ATOM  253  C   LYS A  67  -21.430  28.910   3.660  1.00 34.52  A C
ATOM  254  O   LYS A  67  -21.423  28.596   4.848  1.00 34.17  A O
ATOM  255  N   HIS A  68  -21.476  28.023   2.672  1.00 35.19  A N
ATOM  256  CA  HIS A  68  -21.529  26.592   2.917  1.00 35.89  A C
ATOM  257  CB  HIS A  68  -22.645  25.942   2.097  1.00 35.28  A C
ATOM  258  CG  HIS A  68  -24.020  26.387   2.478  1.00 34.61  A C
ATOM  259  CD2 HIS A  68  -24.722  27.495   2.145  1.00 34.36  A C
ATOM  260  ND1 HIS A  68  -24.827  25.663   3.328  1.00 34.18  A N
ATOM  261  CE1 HIS A  68  -25.965  26.307   3.505  1.00 34.20  A C
ATOM  262  NE2 HIS A  68  -25.928  27.422   2.798  1.00 34.00  A N
ATOM  263  C   HIS A  68  -20.214  25.976   2.512  1.00 36.91  A C
ATOM  264  O   HIS A  68  -19.699  26.240   1.422  1.00 36.68  A O
ATOM  265  N   VAL A  69  -19.677  25.151   3.399  1.00 38.31  A N
ATOM  266  CA  VAL A  69  -18.422  24.461   3.141  1.00 40.00  A C
ATOM  267  CB  VAL A  69  -17.286  24.997   4.033  1.00 39.98  A C
ATOM  268  CG1 VAL A  69  -15.958  24.527   3.494  1.00 40.26  A C
ATOM  269  CG2 VAL A  69  -17.337  26.523   4.104  1.00 40.71  A C
ATOM  270  C   VAL A  69  -18.616  22.987   3.477  1.00 40.89  A C
ATOM  271  O   VAL A  69  -19.063  22.659   4.573  1.00 40.99  A O
ATOM  272  N   GLU A  70  -18.301  22.104   2.535  1.00 42.36  A N
ATOM  273  CA  GLU A  70  -18.420  20.666   2.776  1.00 43.87  A C
ATOM  274  CB  GLU A  70  -18.400  19.894   1.454  1.00 44.27  A C
ATOM  275  CG  GLU A  70  -19.759  19.742   0.803  1.00 45.30  A C
ATOM  276  CD  GLU A  70  -19.686  19.046  -0.551  1.00 46.08  A C
ATOM  277  OE1 GLU A  70  -18.990  18.007  -0.650  1.00 46.54  A O
ATOM  278  OE2 GLU A  70  -20.332  19.528  -1.514  1.00 46.11  A O
```

FIGURE 2A-6

```
ATOM  279  C   GLU A  70  -17.234  20.250   3.633  1.00 44.66  A C
ATOM  280  O   GLU A  70  -16.110  20.675   3.381  1.00 44.49  A O
ATOM  281  N   LYS A  71  -17.479  19.431   4.651  1.00 45.90  A N
ATOM  282  CA  LYS A  71  -16.400  18.992   5.529  1.00 47.31  A C
ATOM  283  CB  LYS A  71  -16.949  18.126   6.658  1.00 46.85  A C
ATOM  284  CG  LYS A  71  -17.920  18.850   7.558  1.00 46.43  A C
ATOM  285  CD  LYS A  71  -18.305  17.982   8.729  1.00 46.14  A C
ATOM  286  CE  LYS A  71  -19.343  18.652   9.590  1.00 45.89  A C
ATOM  287  NZ  LYS A  71  -19.714  17.797  10.737  1.00 45.59  A N
ATOM  288  C   LYS A  71  -15.286  18.240   4.804  1.00 48.59  A C
ATOM  289  O   LYS A  71  -14.116  18.375   5.157  1.00 48.66  A O
ATOM  290  N   ASP A  72  -15.633  17.459   3.787  1.00 50.27  A N
ATOM  291  CA  ASP A  72  -14.611  16.716   3.063  1.00 52.14  A C
ATOM  292  CB  ASP A  72  -15.238  15.718   2.082  1.00 52.48  A C
ATOM  293  CG  ASP A  72  -15.959  14.573   2.785  1.00 53.21  A C
ATOM  294  OD1 ASP A  72  -15.439  14.072   3.809  1.00 53.55  A O
ATOM  295  OD2 ASP A  72  -17.042  14.160   2.304  1.00 53.54  A O
ATOM  296  C   ASP A  72  -13.668  17.625   2.295  1.00 53.32  A C
ATOM  297  O   ASP A  72  -12.601  17.193   1.872  1.00 53.54  A O
ATOM  298  N   ARG A  73  -14.042  18.888   2.130  1.00 54.74  A N
ATOM  299  CA  ARG A  73  -13.214  19.810   1.362  1.00 56.06  A C
ATOM  300  CB  ARG A  73  -14.088  20.604   0.388  1.00 56.50  A C
ATOM  301  CG  ARG A  73  -14.924  19.733  -0.536  1.00 57.29  A C
ATOM  302  CD  ARG A  73  -15.725  20.577  -1.518  1.00 58.16  A C
ATOM  303  NE  ARG A  73  -16.679  19.784  -2.294  1.00 58.87  A N
ATOM  304  CZ  ARG A  73  -17.522  20.295  -3.189  1.00 59.30  A C
ATOM  305  NH1 ARG A  73  -18.363  19.508  -3.857  1.00 59.21  A N
ATOM  306  NH2 ARG A  73  -17.524  21.603  -3.417  1.00 59.81  A N
ATOM  307  C   ARG A  73  -12.353  20.775   2.154  1.00 56.75  A C
ATOM  308  O   ARG A  73  -11.815  21.726   1.585  1.00 56.86  A O
ATOM  309  N   ILE A  74  -12.208  20.546   3.453  1.00 57.56  A N
ATOM  310  CA  ILE A  74  -11.385  21.438   4.263  1.00 58.53  A C
ATOM  311  CB  ILE A  74  -12.231  22.189   5.318  1.00 58.60  A C
ATOM  312  CG2 ILE A  74  -13.104  23.224   4.629  1.00 58.81  A C
ATOM  313  CG1 ILE A  74  -13.096  21.208   6.107  1.00 58.64  A C
ATOM  314  CD1 ILE A  74  -14.107  21.874   7.020  1.00 58.46  A C
ATOM  315  C   ILE A  74  -10.237  20.724   4.960  1.00 59.19  A C
ATOM  316  O   ILE A  74  -10.450  19.818   5.766  1.00 59.25  A O
ATOM  317  N   SER A  75   -9.016  21.152   4.644  1.00 59.89  A N
ATOM  318  CA  SER A  75   -7.809  20.567   5.220  1.00 60.47  A C
ATOM  319  CB  SER A  75   -6.652  20.725   4.246  1.00 60.82  A C
ATOM  320  OG  SER A  75   -6.383  22.103   4.038  1.00 61.38  A O
ATOM  321  C   SER A  75   -7.405  21.198   6.551  1.00 60.76  A C
ATOM  322  O   SER A  75   -6.926  20.505   7.457  1.00 60.92  A O
ATOM  323  N   ASP A  76   -7.589  22.510   6.671  1.00 60.92  A N
ATOM  324  CA  ASP A  76   -7.209  23.202   7.894  1.00 61.04  A C
ATOM  325  CB  ASP A  76   -6.692  24.602   7.574  1.00 61.37  A C
ATOM  326  CG  ASP A  76   -5.366  24.581   6.838  1.00 61.74  A C
ATOM  327  OD1 ASP A  76   -4.659  25.613   6.865  1.00 61.86  A O
ATOM  328  OD2 ASP A  76   -5.033  23.541   6.227  1.00 62.00  A O
ATOM  329  C   ASP A  76   -8.312  23.308   8.923  1.00 60.97  A C
ATOM  330  O   ASP A  76   -9.289  24.018   8.727  1.00 61.09  A O
ATOM  331  N   TRP A  77   -8.144  22.605  10.033  1.00 60.89  A N
ATOM  332  CA  TRP A  77   -9.127  22.645  11.099  1.00 60.78  A C
ATOM  333  CB  TRP A  77   -9.537  21.234  11.519  1.00 60.45  A C
ATOM  334  CG  TRP A  77  -10.025  20.394  10.390  1.00 60.09  A C
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FIGURE 2A-7

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ATOM  335  CD2 TRP A  77  -11.385  20.076  10.084  1.00 59.81  A C
ATOM  336  CE2 TRP A  77  -11.371  19.253   8.937  1.00 59.71  A C
ATOM  337  CE3 TRP A  77  -12.617  20.405  10.668  1.00 59.60  A C
ATOM  338  CD1 TRP A  77   -9.264  19.774   9.445  1.00 59.93  A C
ATOM  339  NE1 TRP A  77  -10.063  19.085   8.569  1.00 59.73  A N
ATOM  340  CZ2 TRP A  77  -12.537  18.750   8.361  1.00 59.76  A C
ATOM  341  CZ3 TRP A  77  -13.783  19.904  10.095  1.00 59.65  A C
ATOM  342  CH2 TRP A  77  -13.732  19.084   8.952  1.00 59.77  A C
ATOM  343  C   TRP A  77   -8.513  23.362  12.278  1.00 60.90  A C
ATOM  344  O   TRP A  77   -7.346  23.153  12.600  1.00 61.00  A O
ATOM  345  N   GLY A  78   -9.299  24.215  12.918  1.00 61.07  A N
ATOM  346  CA  GLY A  78   -8.799  24.945  14.061  1.00 61.42  A C
ATOM  347  C   GLY A  78   -9.405  24.381  15.321  1.00 61.62  A C
ATOM  348  O   GLY A  78  -10.061  23.340  15.282  1.00 61.78  A O
ATOM  349  N   ALA A  79   -9.190  25.068  16.438  1.00 61.73  A N
ATOM  350  CA  ALA A  79   -9.722  24.634  17.721  1.00 61.83  A C
ATOM  351  CB  ALA A  79   -8.580  24.194  18.641  1.00 62.02  A C
ATOM  352  C   ALA A  79  -10.510  25.762  18.365  1.00 61.82  A C
ATOM  353  O   ALA A  79  -11.682  25.595  18.700  1.00 61.94  A O
ATOM  354  N   THR A  84  -14.032  22.352  20.209  1.00 55.01  A N
ATOM  355  CA  THR A  84  -14.503  21.591  19.052  1.00 55.04  A C
ATOM  356  CB  THR A  84  -16.007  21.811  18.832  1.00 55.22  A C
ATOM  357  OG1 THR A  84  -16.336  23.168  19.155  1.00 55.51  A O
ATOM  358  CG2 THR A  84  -16.826  20.861  19.708  1.00 55.41  A C
ATOM  359  C   THR A  84  -13.767  21.927  17.754  1.00 54.81  A C
ATOM  360  O   THR A  84  -13.342  23.064  17.537  1.00 55.01  A O
ATOM  361  N   ARG A  85  -13.624  20.923  16.893  1.00 54.44  A N
ATOM  362  CA  ARG A  85  -12.940  21.074  15.611  1.00 53.97  A C
ATOM  363  CB  ARG A  85  -12.596  19.696  15.034  1.00 54.65  A C
ATOM  364  CG  ARG A  85  -11.117  19.328  15.083  1.00 55.59  A C
ATOM  365  CD  ARG A  85  -10.925  17.824  14.869  1.00 56.41  A C
ATOM  366  NE  ARG A  85  -11.457  17.338  13.592  1.00 57.05  A N
ATOM  367  CZ  ARG A  85  -10.772  17.298  12.452  1.00 57.22  A C
ATOM  368  NH1 ARG A  85   -9.513  17.715  12.412  1.00 57.38  A N
ATOM  369  NH2 ARG A  85  -11.344  16.827  11.351  1.00 57.40  A N
ATOM  370  C   ARG A  85  -13.822  21.827  14.625  1.00 53.23  A C
ATOM  371  O   ARG A  85  -14.961  21.437  14.368  1.00 53.19  A O
ATOM  372  N   VAL A  86  -13.293  22.908  14.068  1.00 52.13  A N
ATOM  373  CA  VAL A  86  -14.050  23.710  13.114  1.00 50.76  A C
ATOM  374  CB  VAL A  86  -14.654  24.969  13.796  1.00 50.65  A C
ATOM  375  CG1 VAL A  86  -15.601  24.559  14.909  1.00 50.45  A C
ATOM  376  CG2 VAL A  86  -13.540  25.842  14.362  1.00 50.51  A C
ATOM  377  C   VAL A  86  -13.085  24.161  12.037  1.00 49.79  A C
ATOM  378  O   VAL A  86  -11.874  24.106  12.230  1.00 49.92  A O
ATOM  379  N   PRO A  87  -13.599  24.587  10.877  1.00 48.80  A N
ATOM  380  CD  PRO A  87  -14.972  24.533  10.351  1.00 48.54  A C
ATOM  381  CA  PRO A  87  -12.656  25.032   9.850  1.00 47.88  A C
ATOM  382  CB  PRO A  87  -13.564  25.352   8.654  1.00 48.06  A C
ATOM  383  CG  PRO A  87  -14.918  25.560   9.261  1.00 48.23  A C
ATOM  384  C   PRO A  87  -11.847  26.241  10.339  1.00 46.97  A C
ATOM  385  O   PRO A  87  -12.386  27.141  10.989  1.00 46.90  A O
ATOM  386  N   MET A  88  -10.551  26.248  10.037  1.00 45.91  A N
ATOM  387  CA  MET A  88   -9.664  27.333  10.456  1.00 44.68  A C
ATOM  388  CB  MET A  88   -8.346  27.269   9.679  1.00 45.30  A C
ATOM  389  CG  MET A  88   -7.308  28.280  10.144  1.00 45.70  A C
ATOM  390  SD  MET A  88   -6.866  28.003  11.872  1.00 46.79  A S
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FIGURE 2A-8

```
ATOM  391  CE  MET A  88   -6.391  26.274  11.794  1.00 46.29  A C
ATOM  392  C   MET A  88  -10.311  28.689  10.226  1.00 43.44  A C
ATOM  393  O   MET A  88  -10.157  29.618  11.013  1.00 43.21  A O
ATOM  394  N   GLU A  89  -11.040  28.785   9.129  1.00 42.03  A N
ATOM  395  CA  GLU A  89  -11.715  30.009   8.750  1.00 40.61  A C
ATOM  396  CB  GLU A  89  -12.585  29.699   7.549  1.00 41.03  A C
ATOM  397  CG  GLU A  89  -13.228  30.868   6.902  1.00 41.52  A C
ATOM  398  CD  GLU A  89  -13.997  30.446   5.663  1.00 42.00  A C
ATOM  399  OE1 GLU A  89  -14.537  31.340   4.985  1.00 42.19  A O
ATOM  400  OE2 GLU A  89  -14.053  29.226   5.365  1.00 41.93  A O
ATOM  401  C   GLU A  89  -12.547  30.591   9.897  1.00 39.49  A C
ATOM  402  O   GLU A  89  -12.577  31.806  10.095  1.00 39.29  A O
ATOM  403  N   VAL A  90  -13.231  29.727  10.645  1.00 38.21  A N
ATOM  404  CA  VAL A  90  -14.038  30.186  11.774  1.00 36.90  A C
ATOM  405  CB  VAL A  90  -14.880  29.046  12.380  1.00 36.82  A C
ATOM  406  CG1 VAL A  90  -15.593  29.538  13.630  1.00 36.60  A C
ATOM  407  CG2 VAL A  90  -15.892  28.562  11.374  1.00 36.74  A C
ATOM  408  C   VAL A  90  -13.128  30.756  12.868  1.00 36.07  A C
ATOM  409  O   VAL A  90  -13.424  31.793  13.446  1.00 35.65  A O
ATOM  410  N   VAL A  91  -12.026  30.072  13.155  1.00 35.18  A N
ATOM  411  CA  VAL A  91  -11.096  30.556  14.166  1.00 34.84  A C
ATOM  412  CB  VAL A  91   -9.894  29.606  14.315  1.00 35.00  A C
ATOM  413  CG1 VAL A  91   -8.841  30.236  15.226  1.00 35.09  A C
ATOM  414  CG2 VAL A  91  -10.360  28.276  14.879  1.00 35.26  A C
ATOM  415  C   VAL A  91  -10.582  31.940  13.761  1.00 34.31  A C
ATOM  416  O   VAL A  91  -10.641  32.898  14.535  1.00 34.33  A O
ATOM  417  N   LEU A  92  -10.081  32.024  12.534  1.00 33.56  A N
ATOM  418  CA  LEU A  92   -9.549  33.256  11.980  1.00 33.00  A C
ATOM  419  CB  LEU A  92   -9.141  33.020  10.520  1.00 32.51  A C
ATOM  420  CG  LEU A  92   -7.713  32.549  10.192  1.00 32.18  A C
ATOM  421  CD1 LEU A  92   -7.012  31.958  11.403  1.00 31.53  A C
ATOM  422  CD2 LEU A  92   -7.769  31.567   9.048  1.00 31.77  A C
ATOM  423  C   LEU A  92  -10.538  34.410  12.069  1.00 32.91  A C
ATOM  424  O   LEU A  92  -10.201  35.474  12.578  1.00 32.63  A O
ATOM  425  N   LEU A  93  -11.760  34.191  11.586  1.00 33.05  A N
ATOM  426  CA  LEU A  93  -12.789  35.228  11.598  1.00 33.47  A C
ATOM  427  CB  LEU A  93  -14.053  34.739  10.876  1.00 33.56  A C
ATOM  428  CG  LEU A  93  -14.013  34.692   9.341  1.00 33.94  A C
ATOM  429  CD1 LEU A  93  -15.231  33.928   8.808  1.00 33.80  A C
ATOM  430  CD2 LEU A  93  -13.987  36.112   8.780  1.00 33.68  A C
ATOM  431  C   LEU A  93  -13.146  35.706  12.998  1.00 33.77  A C
ATOM  432  O   LEU A  93  -13.391  36.886  13.203  1.00 33.73  A O
ATOM  433  N   LYS A  94  -13.177  34.798  13.968  1.00 34.45  A N
ATOM  434  CA  LYS A  94  -13.503  35.202  15.334  1.00 35.21  A C
ATOM  435  CB  LYS A  94  -13.636  33.986  16.251  1.00 35.52  A C
ATOM  436  CG  LYS A  94  -14.974  33.270  16.141  1.00 36.06  A C
ATOM  437  CD  LYS A  94  -14.950  31.981  16.945  1.00 36.89  A C
ATOM  438  CE  LYS A  94  -16.340  31.440  17.174  1.00 37.33  A C
ATOM  439  NZ  LYS A  94  -17.144  32.391  18.012  1.00 37.99  A N
ATOM  440  C   LYS A  94  -12.435  36.127  15.878  1.00 35.50  A C
ATOM  441  O   LYS A  94  -12.741  37.068  16.611  1.00 35.68  A O
ATOM  442  N   LYS A  95  -11.181  35.872  15.508  1.00 35.78  A N
ATOM  443  CA  LYS A  95  -10.083  36.701  15.980  1.00 36.18  A C
ATOM  444  CB  LYS A  95   -8.743  36.033  15.647  1.00 35.98  A C
ATOM  445  CG  LYS A  95   -8.494  34.748  16.444  1.00 36.09  A C
ATOM  446  CD  LYS A  95   -7.226  33.993  16.025  1.00 36.13  A C
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FIGURE 2A-9

```
ATOM  447  CE  LYS A  95    -5.959  34.779  16.308  1.00 36.29   A C
ATOM  448  NZ  LYS A  95    -5.821  35.133  17.751  1.00 36.28   A N
ATOM  449  C   LYS A  95   -10.138  38.128  15.416  1.00 36.64   A C
ATOM  450  O   LYS A  95    -9.753  39.086  16.092  1.00 36.69   A O
ATOM  451  N   VAL A  96   -10.656  38.281  14.200  1.00 37.03   A N
ATOM  452  CA  VAL A  96   -10.717  39.601  13.590  1.00 37.73   A C
ATOM  453  CB  VAL A  96   -10.241  39.566  12.130  1.00 37.66   A C
ATOM  454  CG1 VAL A  96    -8.867  38.956  12.043  1.00 37.48   A C
ATOM  455  CG2 VAL A  96   -11.246  38.790  11.279  1.00 37.52   A C
ATOM  456  C   VAL A  96   -12.085  40.258  13.572  1.00 38.49   A C
ATOM  457  O   VAL A  96   -12.190  41.424  13.191  1.00 38.58   A O
ATOM  458  N   SER A  97   -13.129  39.533  13.971  1.00 39.28   A N
ATOM  459  CA  SER A  97   -14.483  40.088  13.929  1.00 40.19   A C
ATOM  460  CB  SER A  97   -15.509  38.958  13.808  1.00 40.00   A C
ATOM  461  OG  SER A  97   -15.458  38.366  12.519  1.00 39.39   A O
ATOM  462  C   SER A  97   -14.897  41.028  15.064  1.00 41.07   A C
ATOM  463  O   SER A  97   -15.915  41.725  14.969  1.00 41.39   A O
ATOM  464  N   SER A  98   -14.126  41.068  16.139  1.00 41.73   A N
ATOM  465  CA  SER A  98   -14.486  41.956  17.233  1.00 42.41   A C
ATOM  466  CB  SER A  98   -13.639  41.631  18.462  1.00 42.78   A C
ATOM  467  OG  SER A  98   -13.859  42.585  19.484  1.00 43.94   A O
ATOM  468  C   SER A  98   -14.282  43.418  16.818  1.00 42.37   A C
ATOM  469  O   SER A  98   -13.293  43.751  16.168  1.00 42.65   A O
ATOM  470  N   GLY A  99   -15.227  44.280  17.182  1.00 42.31   A N
ATOM  471  CA  GLY A  99   -15.118  45.694  16.845  1.00 41.86   A C
ATOM  472  C   GLY A  99   -15.305  45.988  15.371  1.00 41.57   A C
ATOM  473  O   GLY A  99   -15.478  45.067  14.571  1.00 41.87   A O
ATOM  474  N   PHE A 100   -15.275  47.272  15.017  1.00 41.03   A N
ATOM  475  CA  PHE A 100   -15.434  47.713  13.632  1.00 40.33   A C
ATOM  476  CB  PHE A 100   -15.827  49.189  13.582  1.00 40.99   A C
ATOM  477  CG  PHE A 100   -17.192  49.479  14.126  1.00 41.73   A C
ATOM  478  CD1 PHE A 100   -17.406  50.592  14.938  1.00 41.99   A C
ATOM  479  CD2 PHE A 100   -18.273  48.660  13.808  1.00 41.84   A C
ATOM  480  CE1 PHE A 100   -18.681  50.888  15.426  1.00 42.19   A C
ATOM  481  CE2 PHE A 100   -19.549  48.944  14.288  1.00 42.06   A C
ATOM  482  CZ  PHE A 100   -19.754  50.063  15.102  1.00 42.30   A C
ATOM  483  C   PHE A 100   -14.121  47.552  12.894  1.00 39.54   A C
ATOM  484  O   PHE A 100   -13.057  47.666  13.495  1.00 39.72   A O
ATOM  485  N   SER A 101   -14.195  47.296  11.592  1.00 38.36   A N
ATOM  486  CA  SER A 101   -12.994  47.157  10.780  1.00 37.27   A C
ATOM  487  CB  SER A 101   -12.172  45.958  11.244  1.00 37.31   A C
ATOM  488  OG  SER A 101   -12.832  44.745  10.920  1.00 37.09   A O
ATOM  489  C   SER A 101   -13.372  46.975   9.313  1.00 36.44   A C
ATOM  490  O   SER A 101   -14.558  46.894   8.970  1.00 36.24   A O
ATOM  491  N   GLY A 102   -12.357  46.920   8.457  1.00 35.27   A N
ATOM  492  CA  GLY A 102   -12.591  46.726   7.040  1.00 33.84   A C
ATOM  493  C   GLY A 102   -12.633  45.257   6.637  1.00 32.89   A C
ATOM  494  O   GLY A 102   -12.278  44.909   5.516  1.00 32.64   A O
ATOM  495  N   VAL A 103   -13.024  44.373   7.547  1.00 32.12   A N
ATOM  496  CA  VAL A 103   -13.128  42.964   7.186  1.00 31.80   A C
ATOM  497  CB  VAL A 103   -12.074  42.093   7.938  1.00 31.86   A C
ATOM  498  CG1 VAL A 103   -11.738  42.705   9.244  1.00 32.33   A C
ATOM  499  CG2 VAL A 103   -12.595  40.687   8.157  1.00 31.62   A C
ATOM  500  C   VAL A 103   -14.548  42.464   7.450  1.00 31.43   A C
ATOM  501  O   VAL A 103   -15.156  42.823   8.450  1.00 31.27   A O
ATOM  502  N   ILE A 104   -15.091  41.672   6.528  1.00 31.21   A N
```

FIGURE 2A-10

```
ATOM  503  CA  ILE A 104  -16.437  41.129   6.696  1.00 31.16  A C
ATOM  504  CB  ILE A 104  -16.855  40.257   5.487  1.00 31.04  A C
ATOM  505  CG2 ILE A 104  -17.980  39.284   5.883  1.00 30.79  A C
ATOM  506  CG1 ILE A 104  -17.250  41.164   4.319  1.00 30.76  A C
ATOM  507  CD1 ILE A 104  -18.254  42.219   4.672  1.00 30.20  A C
ATOM  508  C   ILE A 104  -16.475  40.285   7.962  1.00 31.51  A C
ATOM  509  O   ILE A 104  -15.673  39.359   8.135  1.00 31.24  A O
ATOM  510  N   ARG A 105  -17.423  40.605   8.838  1.00 32.01  A N
ATOM  511  CA  ARG A 105  -17.551  39.917  10.112  1.00 32.87  A C
ATOM  512  CB  ARG A 105  -18.081  40.917  11.141  1.00 34.12  A C
ATOM  513  CG  ARG A 105  -17.152  42.118  11.283  1.00 36.17  A C
ATOM  514  CD  ARG A 105  -17.761  43.273  12.058  1.00 37.77  A C
ATOM  515  NE  ARG A 105  -17.777  43.036  13.500  1.00 39.50  A N
ATOM  516  CZ  ARG A 105  -18.066  43.975  14.399  1.00 40.13  A C
ATOM  517  NH1 ARG A 105  -18.366  45.211  14.000  1.00 40.23  A N
ATOM  518  NH2 ARG A 105  -18.038  43.685  15.697  1.00 40.33  A N
ATOM  519  C   ARG A 105  -18.385  38.628  10.143  1.00 32.79  A C
ATOM  520  O   ARG A 105  -19.327  38.447   9.363  1.00 32.53  A O
ATOM  521  N   LEU A 106  -18.009  37.731  11.050  1.00 32.73  A N
ATOM  522  CA  LEU A 106  -18.717  36.477  11.239  1.00 33.02  A C
ATOM  523  CB  LEU A 106  -17.792  35.404  11.798  1.00 32.58  A C
ATOM  524  CG  LEU A 106  -18.431  34.019  11.916  1.00 32.64  A C
ATOM  525  CD1 LEU A 106  -18.755  33.497  10.508  1.00 32.96  A C
ATOM  526  CD2 LEU A 106  -17.482  33.064  12.625  1.00 32.62  A C
ATOM  527  C   LEU A 106  -19.819  36.741  12.253  1.00 33.41  A C
ATOM  528  O   LEU A 106  -19.536  37.051  13.401  1.00 33.51  A O
ATOM  529  N   LEU A 107  -21.072  36.612  11.838  1.00 33.88  A N
ATOM  530  CA  LEU A 107  -22.176  36.863  12.750  1.00 34.65  A C
ATOM  531  CB  LEU A 107  -23.394  37.365  11.974  1.00 34.53  A C
ATOM  532  CG  LEU A 107  -23.176  38.691  11.237  1.00 34.41  A C
ATOM  533  CD1 LEU A 107  -24.401  39.048  10.417  1.00 34.44  A C
ATOM  534  CD2 LEU A 107  -22.872  39.778  12.239  1.00 34.23  A C
ATOM  535  C   LEU A 107  -22.548  35.631  13.553  1.00 35.22  A C
ATOM  536  O   LEU A 107  -22.978  35.737  14.700  1.00 35.12  A O
ATOM  537  N   ASP A 108  -22.365  34.460  12.958  1.00 36.06  A N
ATOM  538  CA  ASP A 108  -22.708  33.209  13.624  1.00 36.90  A C
ATOM  539  CB  ASP A 108  -24.205  33.213  13.935  1.00 37.46  A C
ATOM  540  CG  ASP A 108  -24.648  32.029  14.779  1.00 38.23  A C
ATOM  541  OD1 ASP A 108  -23.818  31.423  15.495  1.00 38.69  A O
ATOM  542  OD2 ASP A 108  -25.856  31.722  14.734  1.00 38.50  A O
ATOM  543  C   ASP A 108  -22.357  32.056  12.697  1.00 37.29  A C
ATOM  544  O   ASP A 108  -22.089  32.266  11.514  1.00 37.28  A O
ATOM  545  N   TRP A 109  -22.331  30.842  13.227  1.00 37.91  A N
ATOM  546  CA  TRP A 109  -22.028  29.684  12.395  1.00 38.69  A C
ATOM  547  CB  TRP A 109  -20.515  29.452  12.320  1.00 39.09  A C
ATOM  548  CG  TRP A 109  -19.894  29.175  13.636  1.00 39.90  A C
ATOM  549  CD2 TRP A 109  -19.622  27.890  14.198  1.00 40.32  A C
ATOM  550  CE2 TRP A 109  -19.089  28.103  15.486  1.00 40.37  A C
ATOM  551  CE3 TRP A 109  -19.780  26.574  13.739  1.00 40.84  A C
ATOM  552  CD1 TRP A 109  -19.524  30.090  14.573  1.00 40.10  A C
ATOM  553  NE1 TRP A 109  -19.039  29.456  15.688  1.00 40.22  A N
ATOM  554  CZ2 TRP A 109  -18.710  27.050  16.328  1.00 40.75  A C
ATOM  555  CZ3 TRP A 109  -19.403  25.521  14.576  1.00 41.01  A C
ATOM  556  CH2 TRP A 109  -18.873  25.770  15.859  1.00 40.98  A C
ATOM  557  C   TRP A 109  -22.729  28.428  12.915  1.00 38.94  A C
ATOM  558  O   TRP A 109  -23.078  28.343  14.093  1.00 38.92  A O
```

FIGURE 2A-11

```
ATOM  559  N   PHE A 110  -22.942  27.463  12.023  1.00 39.18  A N
ATOM  560  CA  PHE A 110  -23.613  26.212  12.373  1.00 39.31  A C
ATOM  561  CB  PHE A 110  -25.037  26.165  11.806  1.00 39.30  A C
ATOM  562  CG  PHE A 110  -25.888  27.332  12.186  1.00 39.38  A C
ATOM  563  CD1 PHE A 110  -25.712  28.563  11.572  1.00 39.32  A C
ATOM  564  CD2 PHE A 110  -26.873  27.199  13.163  1.00 39.49  A C
ATOM  565  CE1 PHE A 110  -26.505  29.652  11.921  1.00 39.52  A C
ATOM  566  CE2 PHE A 110  -27.672  28.278  13.522  1.00 39.64  A C
ATOM  567  CZ  PHE A 110  -27.488  29.511  12.899  1.00 39.69  A C
ATOM  568  C   PHE A 110  -22.874  25.026  11.799  1.00 39.34  A C
ATOM  569  O   PHE A 110  -22.283  25.114  10.729  1.00 39.31  A O
ATOM  570  N   GLU A 111  -22.913  23.909  12.508  1.00 39.48  A N
ATOM  571  CA  GLU A 111  -22.278  22.710  11.997  1.00 39.70  A C
ATOM  572  CB  GLU A 111  -21.418  22.042  13.063  1.00 40.04  A C
ATOM  573  CG  GLU A 111  -20.896  20.688  12.640  1.00 40.67  A C
ATOM  574  CD  GLU A 111  -19.868  20.146  13.601  1.00 41.41  A C
ATOM  575  OE1 GLU A 111  -19.837  20.606  14.765  1.00 41.68  A O
ATOM  576  OE2 GLU A 111  -19.091  19.255  13.196  1.00 41.93  A O
ATOM  577  C   GLU A 111  -23.382  21.759  11.551  1.00 39.60  A C
ATOM  578  O   GLU A 111  -24.382  21.581  12.250  1.00 39.69  A O
ATOM  579  N   ARG A 112  -23.215  21.185  10.369  1.00 39.21  A N
ATOM  580  CA  ARG A 112  -24.181  20.238   9.843  1.00 39.07  A C
ATOM  581  CB  ARG A 112  -24.729  20.693   8.489  1.00 38.63  A C
ATOM  582  CG  ARG A 112  -25.865  21.686   8.598  1.00 38.34  A C
ATOM  583  CD  ARG A 112  -26.246  22.214   7.227  1.00 38.34  A C
ATOM  584  NE  ARG A 112  -27.520  22.924   7.249  1.00 38.14  A N
ATOM  585  CZ  ARG A 112  -28.092  23.456   6.174  1.00 38.13  A C
ATOM  586  NH1 ARG A 112  -27.495  23.366   4.988  1.00 38.10  A N
ATOM  587  NH2 ARG A 112  -29.269  24.060   6.280  1.00 37.73  A N
ATOM  588  C   ARG A 112  -23.466  18.908   9.695  1.00 39.19  A C
ATOM  589  O   ARG A 112  -22.231  18.839   9.737  1.00 39.21  A O
ATOM  590  N   PRO A 113  -24.233  17.827   9.525  1.00 39.21  A N
ATOM  591  CD  PRO A 113  -25.705  17.716   9.444  1.00 39.33  A C
ATOM  592  CA  PRO A 113  -23.594  16.524   9.383  1.00 39.13  A C
ATOM  593  CB  PRO A 113  -24.740  15.636   8.891  1.00 39.39  A C
ATOM  594  CG  PRO A 113  -25.936  16.218   9.627  1.00 39.29  A C
ATOM  595  C   PRO A 113  -22.400  16.532   8.431  1.00 39.06  A C
ATOM  596  O   PRO A 113  -21.300  16.162   8.819  1.00 39.14  A O
ATOM  597  N   ASP A 114  -22.609  16.982   7.197  1.00 38.70  A N
ATOM  598  CA  ASP A 114  -21.540  16.974   6.211  1.00 38.37  A C
ATOM  599  CB  ASP A 114  -22.022  16.212   4.978  1.00 39.38  A C
ATOM  600  CG  ASP A 114  -22.562  14.832   5.332  1.00 40.35  A C
ATOM  601  OD1 ASP A 114  -21.793  14.039   5.924  1.00 41.11  A O
ATOM  602  OD2 ASP A 114  -23.748  14.543   5.032  1.00 40.78  A O
ATOM  603  C   ASP A 114  -20.985  18.332   5.793  1.00 37.67  A C
ATOM  604  O   ASP A 114  -20.269  18.432   4.795  1.00 37.73  A O
ATOM  605  N   SER A 115  -21.295  19.377   6.550  1.00 36.60  A N
ATOM  606  CA  SER A 115  -20.792  20.695   6.199  1.00 35.59  A C
ATOM  607  CB  SER A 115  -21.556  21.235   4.989  1.00 35.38  A C
ATOM  608  OG  SER A 115  -22.868  21.621   5.370  1.00 34.97  A O
ATOM  609  C   SER A 115  -20.914  21.700   7.334  1.00 34.97  A C
ATOM  610  O   SER A 115  -21.532  21.431   8.368  1.00 34.57  A O
ATOM  611  N   PHE A 116  -20.307  22.864   7.120  1.00 34.29  A N
ATOM  612  CA  PHE A 116  -20.374  23.963   8.074  1.00 33.70  A C
ATOM  613  CB  PHE A 116  -18.984  24.389   8.555  1.00 33.83  A C
ATOM  614  CG  PHE A 116  -18.398  23.492   9.608  1.00 34.03  A C
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FIGURE 2A-12

```
ATOM  615  CD1 PHE A 116  -17.595  22.416   9.252  1.00 33.94  A C
ATOM  616  CD2 PHE A 116  -18.627  23.748  10.962  1.00 34.05  A C
ATOM  617  CE1 PHE A 116  -17.018  21.609  10.225  1.00 34.19  A C
ATOM  618  CE2 PHE A 116  -18.055  22.945  11.950  1.00 34.09  A C
ATOM  619  CZ  PHE A 116  -17.249  21.876  11.581  1.00 34.16  A C
ATOM  620  C   PHE A 116  -21.013  25.136   7.358  1.00 33.12  A C
ATOM  621  O   PHE A 116  -20.787  25.341   6.171  1.00 33.09  A O
ATOM  622  N   VAL A 117  -21.812  25.901   8.084  1.00 32.45  A N
ATOM  623  CA  VAL A 117  -22.470  27.058   7.521  1.00 31.89  A C
ATOM  624  CB  VAL A 117  -24.013  26.901   7.556  1.00 32.02  A C
ATOM  625  CG1 VAL A 117  -24.673  28.117   6.927  1.00 31.74  A C
ATOM  626  CG2 VAL A 117  -24.431  25.622   6.808  1.00 32.06  A C
ATOM  627  C   VAL A 117  -22.072  28.298   8.317  1.00 31.56  A C
ATOM  628  O   VAL A 117  -22.214  28.343   9.537  1.00 31.13  A O
ATOM  629  N   LEU A 118  -21.546  29.298   7.618  1.00 31.34  A N
ATOM  630  CA  LEU A 118  -21.140  30.549   8.255  1.00 30.93  A C
ATOM  631  CB  LEU A 118  -19.696  30.907   7.887  1.00 31.05  A C
ATOM  632  CG  LEU A 118  -18.534  30.213   8.610  1.00 31.05  A C
ATOM  633  CD1 LEU A 118  -18.587  28.734   8.361  1.00 31.25  A C
ATOM  634  CD2 LEU A 118  -17.207  30.782   8.114  1.00 30.81  A C
ATOM  635  C   LEU A 118  -22.056  31.682   7.831  1.00 30.62  A C
ATOM  636  O   LEU A 118  -22.351  31.856   6.646  1.00 30.45  A O
ATOM  637  N   ILE A 119  -22.512  32.446   8.811  1.00 30.45  A N
ATOM  638  CA  ILE A 119  -23.376  33.577   8.549  1.00 30.67  A C
ATOM  639  CB  ILE A 119  -24.457  33.726   9.639  1.00 30.64  A C
ATOM  640  CG2 ILE A 119  -25.346  34.901   9.311  1.00 30.60  A C
ATOM  641  CG1 ILE A 119  -25.297  32.443   9.729  1.00 30.66  A C
ATOM  642  CD1 ILE A 119  -26.075  32.115   8.452  1.00 30.87  A C
ATOM  643  C   ILE A 119  -22.449  34.781   8.560  1.00 30.93  A C
ATOM  644  O   ILE A 119  -21.815  35.087   9.569  1.00 31.06  A O
ATOM  645  N   LEU A 120  -22.365  35.453   7.423  1.00 31.23  A N
ATOM  646  CA  LEU A 120  -21.482  36.597   7.271  1.00 31.60  A C
ATOM  647  CB  LEU A 120  -20.576  36.380   6.058  1.00 30.95  A C
ATOM  648  CG  LEU A 120  -19.188  35.762   6.174  1.00 30.88  A C
ATOM  649  CD1 LEU A 120  -18.974  35.044   7.472  1.00 30.93  A C
ATOM  650  CD2 LEU A 120  -18.994  34.851   4.997  1.00 30.81  A C
ATOM  651  C   LEU A 120  -22.221  37.899   7.082  1.00 32.18  A C
ATOM  652  O   LEU A 120  -23.319  37.937   6.543  1.00 32.32  A O
ATOM  653  N   GLU A 121  -21.586  38.974   7.513  1.00 33.05  A N
ATOM  654  CA  GLU A 121  -22.124  40.313   7.363  1.00 33.94  A C
ATOM  655  CB  GLU A 121  -21.144  41.293   8.014  1.00 34.67  A C
ATOM  656  CG  GLU A 121  -21.410  42.767   7.812  1.00 36.60  A C
ATOM  657  CD  GLU A 121  -20.232  43.632   8.267  1.00 37.60  A C
ATOM  658  OE1 GLU A 121  -19.384  43.124   9.037  1.00 38.07  A O
ATOM  659  OE2 GLU A 121  -20.159  44.820   7.856  1.00 38.28  A O
ATOM  660  C   GLU A 121  -22.228  40.582   5.858  1.00 33.99  A C
ATOM  661  O   GLU A 121  -21.428  40.057   5.087  1.00 34.01  A O
ATOM  662  N   ARG A 122  -23.227  41.356   5.435  1.00 34.19  A N
ATOM  663  CA  ARG A 122  -23.370  41.703   4.019  1.00 34.49  A C
ATOM  664  CB  ARG A 122  -24.358  40.790   3.277  1.00 34.48  A C
ATOM  665  CG  ARG A 122  -24.607  41.257   1.820  1.00 34.21  A C
ATOM  666  CD  ARG A 122  -25.413  40.266   0.960  1.00 34.35  A C
ATOM  667  NE  ARG A 122  -26.796  40.060   1.406  1.00 34.16  A N
ATOM  668  CZ  ARG A 122  -27.833  40.825   1.062  1.00 34.07  A C
ATOM  669  NH1 ARG A 122  -27.670  41.870   0.259  1.00 33.41  A N
ATOM  670  NH2 ARG A 122  -29.043  40.536   1.525  1.00 33.88  A N
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FIGURE 2A-13

```
ATOM  671  C   ARG A 122  -23.813  43.144   3.798  1.00 34.69  A C
ATOM  672  O   ARG A 122  -24.970  43.492   4.020  1.00 34.71  A O
ATOM  673  N   PRO A 123  -22.888  44.008   3.368  1.00 34.85  A N
ATOM  674  CD  PRO A 123  -21.425  43.827   3.251  1.00 34.89  A C
ATOM  675  CA  PRO A 123  -23.276  45.401   3.133  1.00 34.79  A C
ATOM  676  CB  PRO A 123  -21.930  46.124   3.070  1.00 35.07  A C
ATOM  677  CG  PRO A 123  -21.002  45.074   2.511  1.00 35.17  A C
ATOM  678  C   PRO A 123  -24.060  45.480   1.823  1.00 34.69  A C
ATOM  679  O   PRO A 123  -24.087  44.518   1.054  1.00 34.34  A O
ATOM  680  N   GLU A 124  -24.713  46.609   1.579  1.00 34.77  A N
ATOM  681  CA  GLU A 124  -25.489  46.784   0.348  1.00 35.02  A C
ATOM  682  CB  GLU A 124  -26.862  46.094   0.459  1.00 36.04  A C
ATOM  683  CG  GLU A 124  -27.581  46.337   1.777  1.00 37.93  A C
ATOM  684  CD  GLU A 124  -29.034  45.844   1.789  1.00 39.23  A C
ATOM  685  OE1 GLU A 124  -29.344  44.767   1.201  1.00 39.72  A O
ATOM  686  OE2 GLU A 124  -29.868  46.546   2.410  1.00 39.79  A O
ATOM  687  C   GLU A 124  -25.691  48.262   0.047  1.00 34.31  A C
ATOM  688  O   GLU A 124  -25.906  49.061   0.964  1.00 34.48  A O
ATOM  689  N   PRO A 125  -25.585  48.656  -1.237  1.00 33.33  A N
ATOM  690  CD  PRO A 125  -25.800  50.054  -1.662  1.00 33.19  A C
ATOM  691  CA  PRO A 125  -25.286  47.807  -2.393  1.00 32.63  A C
ATOM  692  CB  PRO A 125  -25.786  48.647  -3.560  1.00 32.64  A C
ATOM  693  CG  PRO A 125  -25.391  50.030  -3.125  1.00 32.70  A C
ATOM  694  C   PRO A 125  -23.774  47.553  -2.470  1.00 32.07  A C
ATOM  695  O   PRO A 125  -22.976  48.376  -2.018  1.00 32.01  A O
ATOM  696  N   VAL A 126  -23.388  46.439  -3.084  1.00 31.29  A N
ATOM  697  CA  VAL A 126  -21.988  46.066  -3.170  1.00 30.60  A C
ATOM  698  CB  VAL A 126  -21.651  44.989  -2.093  1.00 30.57  A C
ATOM  699  CG1 VAL A 126  -20.239  44.437  -2.296  1.00 30.71  A C
ATOM  700  CG2 VAL A 126  -21.798  45.581  -0.714  1.00 30.38  A C
ATOM  701  C   VAL A 126  -21.599  45.495  -4.518  1.00 30.03  A C
ATOM  702  O   VAL A 126  -22.437  44.940  -5.236  1.00 30.30  A O
ATOM  703  N   GLN A 127  -20.320  45.649  -4.845  1.00 28.98  A N
ATOM  704  CA  GLN A 127  -19.726  45.106  -6.056  1.00 28.19  A C
ATOM  705  CB  GLN A 127  -19.652  46.150  -7.174  1.00 27.89  A C
ATOM  706  CG  GLN A 127  -19.255  45.512  -8.500  1.00 27.90  A C
ATOM  707  CD  GLN A 127  -19.174  46.488  -9.655  1.00 28.17  A C
ATOM  708  OE1 GLN A 127  -19.439  46.124 -10.810  1.00 28.40  A O
ATOM  709  NE2 GLN A 127  -18.794  47.724  -9.364  1.00 27.53  A N
ATOM  710  C   GLN A 127  -18.305  44.719  -5.633  1.00 27.84  A C
ATOM  711  O   GLN A 127  -17.663  45.480  -4.910  1.00 27.39  A O
ATOM  712  N   ASP A 128  -17.813  43.550  -6.046  1.00 27.59  A N
ATOM  713  CA  ASP A 128  -16.456  43.186  -5.659  1.00 27.34  A C
ATOM  714  CB  ASP A 128  -16.230  41.660  -5.766  1.00 27.80  A C
ATOM  715  CG  ASP A 128  -16.163  41.135  -7.197  1.00 28.21  A C
ATOM  716  OD1 ASP A 128  -16.262  39.900  -7.340  1.00 28.62  A O
ATOM  717  OD2 ASP A 128  -15.994  41.905  -8.169  1.00 28.57  A O
ATOM  718  C   ASP A 128  -15.473  44.010  -6.504  1.00 27.10  A C
ATOM  719  O   ASP A 128  -15.857  44.545  -7.548  1.00 26.77  A O
ATOM  720  N   LEU A 129  -14.231  44.156  -6.037  1.00 26.87  A N
ATOM  721  CA  LEU A 129  -13.234  44.957  -6.750  1.00 26.56  A C
ATOM  722  CB  LEU A 129  -11.922  45.015  -5.965  1.00 26.28  A C
ATOM  723  CG  LEU A 129  -11.112  46.320  -5.887  1.00 26.39  A C
ATOM  724  CD1 LEU A 129   -9.676  46.018  -5.463  1.00 25.84  A C
ATOM  725  CD2 LEU A 129  -11.120  47.037  -7.202  1.00 26.46  A C
ATOM  726  C   LEU A 129  -12.949  44.416  -8.141  1.00 26.64  A C
```

FIGURE 2A-14

```
ATOM   727  O   LEU A 129  -12.657  45.168  -9.073  1.00 26.09  A O
ATOM   728  N   PHE A 130  -13.021  43.105  -8.289  1.00 27.17  A N
ATOM   729  CA  PHE A 130  -12.749  42.511  -9.595  1.00 27.99  A C
ATOM   730  CB  PHE A 130  -12.849  40.990  -9.521  1.00 28.39  A C
ATOM   731  CG  PHE A 130  -12.559  40.303 -10.822  1.00 29.22  A C
ATOM   732  CD1 PHE A 130  -11.255  40.020 -11.200  1.00 29.28  A C
ATOM   733  CD2 PHE A 130  -13.597  39.943 -11.677  1.00 29.49  A C
ATOM   734  CE1 PHE A 130  -10.986  39.387 -12.417  1.00 29.75  A C
ATOM   735  CE2 PHE A 130  -13.339  39.310 -12.896  1.00 29.64  A C
ATOM   736  CZ  PHE A 130  -12.033  39.032 -13.265  1.00 29.74  A C
ATOM   737  C   PHE A 130  -13.727  43.041 -10.641  1.00 28.02  A C
ATOM   738  O   PHE A 130  -13.313  43.526 -11.696  1.00 28.02  A O
ATOM   739  N   ASP A 131  -15.025  42.955 -10.342  1.00 28.08  A N
ATOM   740  CA  ASP A 131  -16.051  43.435 -11.269  1.00 28.00  A C
ATOM   741  CB  ASP A 131  -17.451  43.148 -10.733  1.00 27.93  A C
ATOM   742  CG  ASP A 131  -17.791  41.697 -10.762  1.00 27.83  A C
ATOM   743  OD1 ASP A 131  -17.000  40.901 -11.311  1.00 28.42  A O
ATOM   744  OD2 ASP A 131  -18.855  41.346 -10.235  1.00 28.38  A O
ATOM   745  C   ASP A 131  -15.942  44.929 -11.520  1.00 27.87  A C
ATOM   746  O   ASP A 131  -16.134  45.395 -12.648  1.00 27.99  A O
ATOM   747  N   PHE A 132  -15.654  45.678 -10.461  1.00 27.74  A N
ATOM   748  CA  PHE A 132  -15.532  47.122 -10.565  1.00 27.76  A C
ATOM   749  CB  PHE A 132  -15.323  47.706  -9.165  1.00 27.40  A C
ATOM   750  CG  PHE A 132  -15.245  49.206  -9.125  1.00 27.37  A C
ATOM   751  CD1 PHE A 132  -14.028  49.862  -9.321  1.00 27.25  A C
ATOM   752  CD2 PHE A 132  -16.378  49.965  -8.873  1.00 27.22  A C
ATOM   753  CE1 PHE A 132  -13.948  51.257  -9.260  1.00 27.03  A C
ATOM   754  CE2 PHE A 132  -16.306  51.354  -8.812  1.00 27.10  A C
ATOM   755  CZ  PHE A 132  -15.092  52.001  -9.004  1.00 26.79  A C
ATOM   756  C   PHE A 132  -14.389  47.475 -11.527  1.00 28.30  A C
ATOM   757  O   PHE A 132  -14.547  48.331 -12.387  1.00 28.07  A O
ATOM   758  N   ILE A 133  -13.255  46.785 -11.427  1.00 28.73  A N
ATOM   759  CA  ILE A 133  -12.143  47.069 -12.330  1.00 29.51  A C
ATOM   760  CB  ILE A 133  -10.820  46.462 -11.782  1.00 28.91  A C
ATOM   761  CG2 ILE A 133   -9.747  46.478 -12.843  1.00 28.85  A C
ATOM   762  CG1 ILE A 133  -10.362  47.256 -10.559  1.00 28.66  A C
ATOM   763  CD1 ILE A 133   -9.219  46.629  -9.781  1.00 28.30  A C
ATOM   764  C   ILE A 133  -12.427  46.569 -13.765  1.00 30.48  A C
ATOM   765  O   ILE A 133  -12.010  47.196 -14.747  1.00 30.46  A O
ATOM   766  N   THR A 134  -13.135  45.450 -13.895  1.00 31.43  A N
ATOM   767  CA  THR A 134  -13.468  44.932 -15.221  1.00 32.53  A C
ATOM   768  CB  THR A 134  -14.183  43.562 -15.115  1.00 32.56  A C
ATOM   769  OG1 THR A 134  -13.296  42.605 -14.520  1.00 32.82  A O
ATOM   770  CG2 THR A 134  -14.607  43.061 -16.491  1.00 32.45  A C
ATOM   771  C   THR A 134  -14.380  45.929 -15.966  1.00 33.35  A C
ATOM   772  O   THR A 134  -14.239  46.137 -17.168  1.00 33.60  A O
ATOM   773  N   GLU A 135  -15.302  46.563 -15.251  1.00 34.33  A N
ATOM   774  CA  GLU A 135  -16.206  47.517 -15.883  1.00 35.30  A C
ATOM   775  CB  GLU A 135  -17.483  47.667 -15.055  1.00 36.19  A C
ATOM   776  CG  GLU A 135  -18.297  46.375 -14.986  1.00 37.87  A C
ATOM   777  CD  GLU A 135  -19.604  46.544 -14.239  1.00 38.91  A C
ATOM   778  OE1 GLU A 135  -20.334  45.533 -14.113  1.00 39.56  A O
ATOM   779  OE2 GLU A 135  -19.897  47.681 -13.783  1.00 39.16  A O
ATOM   780  C   GLU A 135  -15.596  48.896 -16.111  1.00 35.43  A C
ATOM   781  O   GLU A 135  -15.851  49.539 -17.133  1.00 35.27  A O
ATOM   782  N   ARG A 136  -14.783  49.352 -15.168  1.00 35.14  A N
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FIGURE 2A-15

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ATOM  783  CA  ARG A 136  -14.186  50.665 -15.302  1.00 34.79  A C
ATOM  784  CB  ARG A 136  -14.171  51.355 -13.952  1.00 35.73  A C
ATOM  785  CG  ARG A 136  -15.540  51.687 -13.409  1.00 36.89  A C
ATOM  786  CD  ARG A 136  -15.406  52.944 -12.562  1.00 38.05  A C
ATOM  787  NE  ARG A 136  -16.626  53.280 -11.845  1.00 38.72  A N
ATOM  788  CZ  ARG A 136  -16.766  54.376 -11.110  1.00 39.04  A C
ATOM  789  NH1 ARG A 136  -15.757  55.238 -11.009  1.00 38.90  A N
ATOM  790  NH2 ARG A 136  -17.907  54.596 -10.466  1.00 39.24  A N
ATOM  791  C   ARG A 136  -12.779  50.709 -15.879  1.00 34.01  A C
ATOM  792  O   ARG A 136  -12.303  51.780 -16.258  1.00 33.91  A O
ATOM  793  N   GLY A 137  -12.108  49.563 -15.947  1.00 33.27  A N
ATOM  794  CA  GLY A 137  -10.743  49.549 -16.451  1.00 32.29  A C
ATOM  795  C   GLY A 137   -9.830  50.158 -15.392  1.00 31.65  A C
ATOM  796  O   GLY A 137  -10.206  50.218 -14.221  1.00 31.68  A O
ATOM  797  N   ALA A 138   -8.650  50.631 -15.784  1.00 30.81  A N
ATOM  798  CA  ALA A 138   -7.719  51.216 -14.823  1.00 30.02  A C
ATOM  799  CB  ALA A 138   -6.494  51.780 -15.549  1.00 29.90  A C
ATOM  800  C   ALA A 138   -8.401  52.311 -13.997  1.00 29.62  A C
ATOM  801  O   ALA A 138   -9.228  53.074 -14.516  1.00 29.65  A O
ATOM  802  N   LEU A 139   -8.047  52.381 -12.715  1.00 28.60  A N
ATOM  803  CA  LEU A 139   -8.625  53.359 -11.806  1.00 28.07  A C
ATOM  804  CB  LEU A 139   -8.825  52.741 -10.418  1.00 27.41  A C
ATOM  805  CG  LEU A 139   -9.512  51.379 -10.260  1.00 27.45  A C
ATOM  806  CD1 LEU A 139   -9.646  51.042  -8.761  1.00 26.68  A C
ATOM  807  CD2 LEU A 139  -10.879  51.402 -10.930  1.00 27.01  A C
ATOM  808  C   LEU A 139   -7.737  54.594 -11.656  1.00 27.82  A C
ATOM  809  O   LEU A 139   -6.507  54.482 -11.657  1.00 27.46  A O
ATOM  810  N   GLN A 140   -8.360  55.767 -11.530  1.00 27.62  A N
ATOM  811  CA  GLN A 140   -7.612  57.001 -11.320  1.00 27.81  A C
ATOM  812  CB  GLN A 140   -8.556  58.193 -11.114  1.00 29.02  A C
ATOM  813  CG  GLN A 140   -9.529  58.391 -12.273  1.00 31.34  A C
ATOM  814  CD  GLN A 140  -10.434  59.602 -12.077  1.00 32.76  A C
ATOM  815  OE1 GLN A 140  -11.440  59.753 -12.778  1.00 34.01  A O
ATOM  816  NE2 GLN A 140  -10.056  60.495 -11.154  1.00 33.05  A N
ATOM  817  C   GLN A 140   -6.806  56.780 -10.044  1.00 27.15  A C
ATOM  818  O   GLN A 140   -7.257  56.086  -9.124  1.00 26.33  A O
ATOM  819  N   GLU A 141   -5.624  57.380  -9.980  1.00 26.89  A N
ATOM  820  CA  GLU A 141   -4.768  57.196  -8.818  1.00 26.91  A C
ATOM  821  CB  GLU A 141   -3.416  57.879  -9.045  1.00 27.02  A C
ATOM  822  CG  GLU A 141   -2.710  57.308 -10.280  1.00 27.85  A C
ATOM  823  CD  GLU A 141   -1.213  57.555 -10.323  1.00 27.69  A C
ATOM  824  OE1 GLU A 141   -0.606  57.267 -11.365  1.00 28.06  A O
ATOM  825  OE2 GLU A 141   -0.635  58.027  -9.329  1.00 28.68  A O
ATOM  826  C   GLU A 141   -5.404  57.638  -7.505  1.00 26.82  A C
ATOM  827  O   GLU A 141   -5.169  57.013  -6.474  1.00 26.63  A O
ATOM  828  N   GLU A 142   -6.224  58.686  -7.543  1.00 26.73  A N
ATOM  829  CA  GLU A 142   -6.887  59.175  -6.336  1.00 26.67  A C
ATOM  830  CB  GLU A 142   -7.725  60.424  -6.651  1.00 27.44  A C
ATOM  831  CG  GLU A 142   -8.559  60.931  -5.482  1.00 28.70  A C
ATOM  832  CD  GLU A 142   -9.275  62.239  -5.792  1.00 29.58  A C
ATOM  833  OE1 GLU A 142   -8.696  63.315  -5.514  1.00 30.25  A O
ATOM  834  OE2 GLU A 142  -10.406  62.189  -6.324  1.00 29.89  A O
ATOM  835  C   GLU A 142   -7.788  58.086  -5.766  1.00 26.11  A C
ATOM  836  O   GLU A 142   -7.861  57.877  -4.551  1.00 26.22  A O
ATOM  837  N   LEU A 143   -8.482  57.395  -6.654  1.00 25.37  A N
ATOM  838  CA  LEU A 143   -9.378  56.326  -6.250  1.00 24.70  A C
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FIGURE 2A-16

```
ATOM  839  CB  LEU A 143   -10.318  55.982  -7.417  1.00 24.13  A C
ATOM  840  CG  LEU A 143   -11.365  54.899  -7.174  1.00 23.61  A C
ATOM  841  CD1 LEU A 143   -12.233  55.256  -5.978  1.00 23.29  A C
ATOM  842  CD2 LEU A 143   -12.201  54.740  -8.431  1.00 23.71  A C
ATOM  843  C   LEU A 143    -8.563  55.101  -5.808  1.00 24.34  A C
ATOM  844  O   LEU A 143    -8.845  54.502  -4.775  1.00 24.32  A O
ATOM  845  N   ALA A 144    -7.538  54.743  -6.579  1.00 24.18  A N
ATOM  846  CA  ALA A 144    -6.696  53.600  -6.217  1.00 23.80  A C
ATOM  847  CB  ALA A 144    -5.603  53.391  -7.266  1.00 23.28  A C
ATOM  848  C   ALA A 144    -6.060  53.840  -4.840  1.00 23.65  A C
ATOM  849  O   ALA A 144    -5.931  52.906  -4.048  1.00 23.41  A O
ATOM  850  N   ARG A 145    -5.677  55.090  -4.560  1.00 23.37  A N
ATOM  851  CA  ARG A 145    -5.038  55.431  -3.282  1.00 23.53  A C
ATOM  852  CB  ARG A 145    -4.576  56.898  -3.270  1.00 23.85  A C
ATOM  853  CG  ARG A 145    -3.951  57.346  -1.939  1.00 24.90  A C
ATOM  854  CD  ARG A 145    -3.069  58.595  -2.104  1.00 26.20  A C
ATOM  855  NE  ARG A 145    -3.763  59.588  -2.899  1.00 27.51  A N
ATOM  856  CZ  ARG A 145    -3.339  60.075  -4.061  1.00 27.28  A C
ATOM  857  NH1 ARG A 145    -2.188  59.680  -4.587  1.00 27.00  A N
ATOM  858  NH2 ARG A 145    -4.111  60.924  -4.719  1.00 27.33  A N
ATOM  859  C   ARG A 145    -5.980  55.177  -2.117  1.00 23.25  A C
ATOM  860  O   ARG A 145    -5.604  54.539  -1.133  1.00 23.05  A O
ATOM  861  N   SER A 146    -7.210  55.669  -2.243  1.00 23.12  A N
ATOM  862  CA  SER A 146    -8.225  55.486  -1.207  1.00 23.05  A C
ATOM  863  CB  SER A 146    -9.504  56.213  -1.602  1.00 23.13  A C
ATOM  864  OG  SER A 146   -10.562  55.852  -0.729  1.00 24.07  A O
ATOM  865  C   SER A 146    -8.536  54.006  -0.983  1.00 22.61  A C
ATOM  866  O   SER A 146    -8.632  53.548   0.156  1.00 22.47  A O
ATOM  867  N   PHE A 147    -8.706  53.271  -2.081  1.00 22.23  A N
ATOM  868  CA  PHE A 147    -8.998  51.847  -2.016  1.00 22.01  A C
ATOM  869  CB  PHE A 147    -9.301  51.307  -3.416  1.00 22.33  A C
ATOM  870  CG  PHE A 147   -10.707  51.565  -3.888  1.00 22.73  A C
ATOM  871  CD1 PHE A 147   -11.183  50.948  -5.043  1.00 22.51  A C
ATOM  872  CD2 PHE A 147   -11.567  52.402  -3.168  1.00 22.92  A C
ATOM  873  CE1 PHE A 147   -12.489  51.151  -5.474  1.00 22.69  A C
ATOM  874  CE2 PHE A 147   -12.880  52.614  -3.594  1.00 23.07  A C
ATOM  875  CZ  PHE A 147   -13.339  51.982  -4.753  1.00 23.07  A C
ATOM  876  C   PHE A 147    -7.810  51.076  -1.421  1.00 21.83  A C
ATOM  877  O   PHE A 147    -7.971  50.272  -0.501  1.00 21.25  A O
ATOM  878  N   PHE A 148    -6.620  51.335  -1.953  1.00 21.29  A N
ATOM  879  CA  PHE A 148    -5.429  50.664  -1.476  1.00 21.53  A C
ATOM  880  CB  PHE A 148    -4.201  51.110  -2.287  1.00 21.33  A C
ATOM  881  CG  PHE A 148    -2.989  50.251  -2.056  1.00 21.35  A C
ATOM  882  CD1 PHE A 148    -3.027  48.879  -2.333  1.00 21.37  A C
ATOM  883  CD2 PHE A 148    -1.814  50.799  -1.570  1.00 21.27  A C
ATOM  884  CE1 PHE A 148    -1.914  48.078  -2.129  1.00 20.70  A C
ATOM  885  CE2 PHE A 148    -0.694  49.996  -1.367  1.00 21.22  A C
ATOM  886  CZ  PHE A 148    -0.749  48.635  -1.648  1.00 20.74  A C
ATOM  887  C   PHE A 148    -5.213  50.947   0.012  1.00 21.51  A C
ATOM  888  O   PHE A 148    -4.889  50.049   0.776  1.00 21.45  A O
ATOM  889  N   TRP A 149    -5.411  52.197   0.418  1.00 21.90  A N
ATOM  890  CA  TRP A 149    -5.251  52.596   1.822  1.00 22.04  A C
ATOM  891  CB  TRP A 149    -5.561  54.085   1.980  1.00 22.07  A C
ATOM  892  CG  TRP A 149    -5.422  54.590   3.385  1.00 22.78  A C
ATOM  893  CD2 TRP A 149    -4.237  55.121   3.992  1.00 23.01  A C
ATOM  894  CE2 TRP A 149    -4.579  55.520   5.302  1.00 23.40  A C
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FIGURE 2A-17

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ATOM  895  CE3 TRP A 149    -2.918  55.303   3.550  1.00 23.62   A C
ATOM  896  CD1 TRP A 149    -6.405  54.677   4.324  1.00 22.84   A C
ATOM  897  NE1 TRP A 149    -5.909  55.238   5.481  1.00 23.12   A N
ATOM  898  CZ2 TRP A 149    -3.648  56.095   6.187  1.00 23.63   A C
ATOM  899  CZ3 TRP A 149    -1.982  55.878   4.435  1.00 24.05   A C
ATOM  900  CH2 TRP A 149    -2.362  56.265   5.740  1.00 23.42   A C
ATOM  901  C   TRP A 149    -6.163  51.785   2.738  1.00 22.12   A C
ATOM  902  O   TRP A 149    -5.726  51.290   3.780  1.00 21.89   A O
ATOM  903  N   GLN A 150    -7.429  51.654   2.344  1.00 22.26   A N
ATOM  904  CA  GLN A 150    -8.392  50.889   3.127  1.00 22.41   A C
ATOM  905  CB  GLN A 150    -9.803  51.043   2.556  1.00 22.54   A C
ATOM  906  CG  GLN A 150   -10.406  52.413   2.770  1.00 22.82   A C
ATOM  907  CD  GLN A 150   -11.848  52.474   2.313  1.00 23.43   A C
ATOM  908  OE1 GLN A 150   -12.697  51.735   2.803  1.00 23.47   A O
ATOM  909  NE2 GLN A 150   -12.129  53.353   1.363  1.00 23.65   A N
ATOM  910  C   GLN A 150    -8.024  49.415   3.181  1.00 22.59   A C
ATOM  911  O   GLN A 150    -8.209  48.767   4.214  1.00 22.53   A O
ATOM  912  N   VAL A 151    -7.519  48.867   2.077  1.00 22.52   A N
ATOM  913  CA  VAL A 151    -7.113  47.466   2.099  1.00 22.70   A C
ATOM  914  CB  VAL A 151    -6.680  46.973   0.690  1.00 22.72   A C
ATOM  915  CG1 VAL A 151    -6.020  45.596   0.771  1.00 22.46   A C
ATOM  916  CG2 VAL A 151    -7.916  46.903  -0.220  1.00 22.47   A C
ATOM  917  C   VAL A 151    -5.956  47.347   3.100  1.00 22.82   A C
ATOM  918  O   VAL A 151    -5.935  46.427   3.918  1.00 22.81   A O
ATOM  919  N   LEU A 152    -5.013  48.288   3.065  1.00 22.73   A N
ATOM  920  CA  LEU A 152    -3.897  48.224   3.997  1.00 22.93   A C
ATOM  921  CB  LEU A 152    -2.924  49.374   3.759  1.00 23.30   A C
ATOM  922  CG  LEU A 152    -1.911  49.149   2.665  1.00 23.90   A C
ATOM  923  CD1 LEU A 152    -1.403  50.460   2.243  1.00 24.55   A C
ATOM  924  CD2 LEU A 152    -0.757  48.293   3.145  1.00 24.86   A C
ATOM  925  C   LEU A 152    -4.378  48.260   5.432  1.00 22.83   A C
ATOM  926  O   LEU A 152    -3.897  47.498   6.257  1.00 23.16   A O
ATOM  927  N   GLU A 153    -5.322  49.143   5.736  1.00 22.70   A N
ATOM  928  CA  GLU A 153    -5.820  49.220   7.104  1.00 23.02   A C
ATOM  929  CB  GLU A 153    -6.823  50.367   7.262  1.00 23.29   A C
ATOM  930  CG  GLU A 153    -6.186  51.754   7.164  1.00 23.74   A C
ATOM  931  CD  GLU A 153    -5.348  52.118   8.387  1.00 24.40   A C
ATOM  932  OE1 GLU A 153    -4.345  52.846   8.225  1.00 24.48   A O
ATOM  933  OE2 GLU A 153    -5.699  51.696   9.512  1.00 24.53   A O
ATOM  934  C   GLU A 153    -6.471  47.901   7.517  1.00 22.98   A C
ATOM  935  O   GLU A 153    -6.323  47.470   8.666  1.00 22.88   A O
ATOM  936  N   ALA A 154    -7.175  47.257   6.583  1.00 22.62   A N
ATOM  937  CA  ALA A 154    -7.842  45.981   6.876  1.00 22.66   A C
ATOM  938  CB  ALA A 154    -8.746  45.573   5.706  1.00 21.87   A C
ATOM  939  C   ALA A 154    -6.816  44.872   7.160  1.00 22.42   A C
ATOM  940  O   ALA A 154    -6.973  44.082   8.094  1.00 22.27   A O
ATOM  941  N   VAL A 155    -5.770  44.828   6.347  1.00 22.30   A N
ATOM  942  CA  VAL A 155    -4.739  43.833   6.508  1.00 22.31   A C
ATOM  943  CB  VAL A 155    -3.797  43.823   5.284  1.00 22.15   A C
ATOM  944  CG1 VAL A 155    -2.674  42.828   5.497  1.00 22.05   A C
ATOM  945  CG2 VAL A 155    -4.603  43.455   4.020  1.00 22.27   A C
ATOM  946  C   VAL A 155    -3.964  44.082   7.801  1.00 22.49   A C
ATOM  947  O   VAL A 155    -3.610  43.132   8.494  1.00 22.68   A O
ATOM  948  N   ARG A 156    -3.708  45.342   8.147  1.00 22.68   A N
ATOM  949  CA  ARG A 156    -2.993  45.623   9.404  1.00 23.10   A C
ATOM  950  CB  ARG A 156    -2.704  47.117   9.562  1.00 23.00   A C
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FIGURE 2A-18

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ATOM   951  CG  ARG A 156    -1.595  47.654   8.660  1.00 23.08   A C
ATOM   952  CD  ARG A 156    -1.428  49.162   8.886  1.00 23.24   A C
ATOM   953  NE  ARG A 156    -1.144  49.441  10.283  1.00 22.74   A N
ATOM   954  CZ  ARG A 156    -1.387  50.597  10.889  1.00 22.80   A C
ATOM   955  NH1 ARG A 156    -1.924  51.608  10.220  1.00 22.84   A N
ATOM   956  NH2 ARG A 156    -1.119  50.725  12.188  1.00 22.72   A N
ATOM   957  C   ARG A 156    -3.832  45.152  10.589  1.00 23.52   A C
ATOM   958  O   ARG A 156    -3.303  44.646  11.576  1.00 23.39   A O
ATOM   959  N   HIS A 157    -5.147  45.323  10.476  1.00 24.13   A N
ATOM   960  CA  HIS A 157    -6.068  44.910  11.521  1.00 24.89   A C
ATOM   961  CB  HIS A 157    -7.504  45.291  11.143  1.00 25.37   A C
ATOM   962  CG  HIS A 157    -8.538  44.704  12.051  1.00 26.01   A C
ATOM   963  CD2 HIS A 157    -9.407  43.679  11.869  1.00 26.49   A C
ATOM   964  ND1 HIS A 157    -8.712  45.129  13.350  1.00 26.55   A N
ATOM   965  CE1 HIS A 157    -9.641  44.388  13.933  1.00 26.77   A C
ATOM   966  NE2 HIS A 157   -10.077  43.501  13.057  1.00 26.95   A N
ATOM   967  C   HIS A 157    -5.968  43.399  11.723  1.00 25.23   A C
ATOM   968  O   HIS A 157    -5.881  42.928  12.859  1.00 24.91   A O
ATOM   969  N   CYS A 158    -5.975  42.640  10.626  1.00 25.47   A N
ATOM   970  CA  CYS A 158    -5.868  41.186  10.728  1.00 25.77   A C
ATOM   971  CB  CYS A 158    -5.938  40.523   9.345  1.00 25.84   A C
ATOM   972  SG  CYS A 158    -7.492  40.682   8.434  1.00 26.06   A S
ATOM   973  C   CYS A 158    -4.542  40.783  11.382  1.00 26.20   A C
ATOM   974  O   CYS A 158    -4.527  39.968  12.307  1.00 25.99   A O
ATOM   975  N   HIS A 159    -3.435  41.328  10.871  1.00 26.76   A N
ATOM   976  CA  HIS A 159    -2.111  41.011  11.401  1.00 27.67   A C
ATOM   977  CB  HIS A 159    -1.020  41.763  10.618  1.00 27.99   A C
ATOM   978  CG  HIS A 159    -0.772  41.221   9.246  1.00 28.87   A C
ATOM   979  CD2 HIS A 159     0.321  41.265   8.452  1.00 29.15   A C
ATOM   980  ND1 HIS A 159    -1.740  40.554   8.522  1.00 29.69   A N
ATOM   981  CE1 HIS A 159    -1.253  40.208   7.347  1.00 29.22   A C
ATOM   982  NE2 HIS A 159    -0.003  40.628   7.277  1.00 29.53   A N
ATOM   983  C   HIS A 159    -2.058  41.415  12.872  1.00 28.14   A C
ATOM   984  O   HIS A 159    -1.470  40.733  13.694  1.00 27.98   A O
ATOM   985  N   ASN A 160    -2.701  42.522  13.196  1.00 28.86   A N
ATOM   986  CA  ASN A 160    -2.688  42.984  14.558  1.00 29.86   A C
ATOM   987  CB  ASN A 160    -3.398  44.322  14.677  1.00 30.87   A C
ATOM   988  CG  ASN A 160    -3.241  44.945  16.042  1.00 32.19   A C
ATOM   989  OD1 ASN A 160    -3.959  45.885  16.382  1.00 33.38   A O
ATOM   990  ND2 ASN A 160    -2.278  44.470  16.817  1.00 32.64   A N
ATOM   991  C   ASN A 160    -3.403  41.977  15.438  1.00 29.85   A C
ATOM   992  O   ASN A 160    -3.140  41.890  16.629  1.00 30.12   A O
ATOM   993  N   CME A 161    -4.337  41.243  14.849  1.00 29.80   A N
ATOM   994  CA  CME A 161    -5.127  40.260  15.569  1.00 29.55   A C
ATOM   995  C   CME A 161    -4.588  38.849  15.406  1.00 28.35   A C
ATOM   996  CB  CME A 161    -6.588  40.321  15.090  1.00 31.48   A C
ATOM   997  SG  CME A 161    -7.474  41.840  15.643  1.00 34.40   A S
ATOM   998  S1  CME A 161    -7.352  41.854  17.770  1.00 37.86   A S
ATOM   999  C1  CME A 161    -6.214  43.203  18.227  1.00 37.87   A C
ATOM  1000  C2  CME A 161    -6.474  43.832  19.605  1.00 39.27   A C
ATOM  1001  O1  CME A 161    -7.859  44.341  19.774  1.00 40.16   A O
ATOM  1002  O   CME A 161    -5.273  37.892  15.736  1.00 27.93   A O
ATOM  1003  N   GLY A 162    -3.373  38.717  14.884  1.00 27.18   A N
ATOM  1004  CA  GLY A 162    -2.783  37.398  14.735  1.00 26.05   A C
ATOM  1005  C   GLY A 162    -3.266  36.556  13.561  1.00 25.55   A C
ATOM  1006  O   GLY A 162    -3.088  35.335  13.569  1.00 25.27   A O
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FIGURE 2A-19

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ATOM 1007  N   VAL A 163   -3.858  37.195  12.548  1.00 24.73  A N
ATOM 1008  CA  VAL A 163   -4.374  36.487  11.372  1.00 24.04  A C
ATOM 1009  CB  VAL A 163   -5.901  36.722  11.202  1.00 24.03  A C
ATOM 1010  CG1 VAL A 163   -6.429  35.931  10.021  1.00 24.06  A C
ATOM 1011  CG2 VAL A 163   -6.635  36.340  12.471  1.00 23.84  A C
ATOM 1012  C   VAL A 163   -3.710  36.917  10.071  1.00 23.75  A C
ATOM 1013  O   VAL A 163   -3.544  38.114   9.803  1.00 23.66  A O
ATOM 1014  N   LEU A 164   -3.351  35.933   9.260  1.00 23.53  A N
ATOM 1015  CA  LEU A 164   -2.735  36.169   7.956  1.00 23.83  A C
ATOM 1016  CB  LEU A 164   -1.455  35.331   7.820  1.00 23.93  A C
ATOM 1017  CG  LEU A 164   -0.553  35.607   6.611  1.00 24.18  A C
ATOM 1018  CD1 LEU A 164    0.058  36.994   6.769  1.00 24.02  A C
ATOM 1019  CD2 LEU A 164    0.553  34.537   6.509  1.00 23.86  A C
ATOM 1020  C   LEU A 164   -3.770  35.715   6.911  1.00 23.79  A C
ATOM 1021  O   LEU A 164   -4.161  34.540   6.893  1.00 23.70  A O
ATOM 1022  N   HIS A 165   -4.222  36.632   6.059  1.00 23.49  A N
ATOM 1023  CA  HIS A 165   -5.227  36.288   5.040  1.00 23.37  A C
ATOM 1024  CB  HIS A 165   -5.720  37.562   4.336  1.00 22.79  A C
ATOM 1025  CG  HIS A 165   -6.879  37.334   3.414  1.00 22.16  A C
ATOM 1026  CD2 HIS A 165   -8.194  37.630   3.550  1.00 21.64  A C
ATOM 1027  ND1 HIS A 165   -6.751  36.713   2.190  1.00 21.78  A N
ATOM 1028  CE1 HIS A 165   -7.937  36.639   1.612  1.00 21.67  A C
ATOM 1029  NE2 HIS A 165   -8.829  37.189   2.417  1.00 21.74  A N
ATOM 1030  C   HIS A 165   -4.752  35.284   3.977  1.00 23.71  A C
ATOM 1031  O   HIS A 165   -5.455  34.306   3.681  1.00 24.00  A O
ATOM 1032  N   ARG A 166   -3.582  35.555   3.394  1.00 23.83  A N
ATOM 1033  CA  ARG A 166   -2.942  34.724   2.361  1.00 24.15  A C
ATOM 1034  CB  ARG A 166   -2.679  33.309   2.901  1.00 24.59  A C
ATOM 1035  CG  ARG A 166   -1.624  33.290   4.019  1.00 25.45  A C
ATOM 1036  CD  ARG A 166   -1.045  31.893   4.266  1.00 26.07  A C
ATOM 1037  NE  ARG A 166   -2.040  30.933   4.734  1.00 26.62  A N
ATOM 1038  CZ  ARG A 166   -1.772  29.655   4.995  1.00 27.27  A C
ATOM 1039  NH1 ARG A 166   -0.533  29.191   4.828  1.00 27.01  A N
ATOM 1040  NH2 ARG A 166   -2.730  28.842   5.439  1.00 27.00  A N
ATOM 1041  C   ARG A 166   -3.598  34.651   0.970  1.00 24.11  A C
ATOM 1042  O   ARG A 166   -3.130  33.927   0.082  1.00 24.10  A O
ATOM 1043  N   ASP A 167   -4.667  35.401   0.757  1.00 23.95  A N
ATOM 1044  CA  ASP A 167   -5.266  35.401  -0.566  1.00 24.06  A C
ATOM 1045  CB  ASP A 167   -6.361  34.337  -0.642  1.00 24.45  A C
ATOM 1046  CG  ASP A 167   -6.821  34.073  -2.059  1.00 25.40  A C
ATOM 1047  OD1 ASP A 167   -6.038  34.298  -3.024  1.00 25.51  A O
ATOM 1048  OD2 ASP A 167   -7.978  33.627  -2.202  1.00 26.01  A O
ATOM 1049  C   ASP A 167   -5.798  36.788  -0.942  1.00 23.71  A C
ATOM 1050  O   ASP A 167   -6.859  36.919  -1.544  1.00 23.57  A O
ATOM 1051  N   ILE A 168   -5.041  37.826  -0.591  1.00 23.53  A N
ATOM 1052  CA  ILE A 168   -5.431  39.196  -0.906  1.00 23.06  A C
ATOM 1053  CB  ILE A 168   -4.439  40.210  -0.311  1.00 22.56  A C
ATOM 1054  CG2 ILE A 168   -4.818  41.633  -0.739  1.00 21.68  A C
ATOM 1055  CG1 ILE A 168   -4.405  40.071   1.213  1.00 21.67  A C
ATOM 1056  CD1 ILE A 168   -3.255  40.823   1.849  1.00 20.82  A C
ATOM 1057  C   ILE A 168   -5.452  39.390  -2.417  1.00 23.41  A C
ATOM 1058  O   ILE A 168   -4.453  39.146  -3.090  1.00 23.37  A O
ATOM 1059  N   LYS A 169   -6.591  39.832  -2.942  1.00 23.53  A N
ATOM 1060  CA  LYS A 169   -6.754  40.079  -4.380  1.00 23.92  A C
ATOM 1061  CB  LYS A 169   -6.668  38.766  -5.173  1.00 24.05  A C
ATOM 1062  CG  LYS A 169   -7.670  37.699  -4.745  1.00 24.69  A C
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FIGURE 2A-20

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ATOM 1063  CD  LYS A 169    -7.669  36.518  -5.726  1.00 25.08  A C
ATOM 1064  CE  LYS A 169    -8.667  35.450  -5.296  1.00 25.61  A C
ATOM 1065  NZ  LYS A 169    -8.604  34.267  -6.208  1.00 26.17  A N
ATOM 1066  C   LYS A 169    -8.114  40.755  -4.615  1.00 24.05  A C
ATOM 1067  O   LYS A 169    -8.980  40.735  -3.729  1.00 23.81  A O
ATOM 1068  N   ASP A 170    -8.302  41.331  -5.800  1.00 24.07  A N
ATOM 1069  CA  ASP A 170    -9.537  42.044  -6.121  1.00 24.31  A C
ATOM 1070  CB  ASP A 170    -9.494  42.594  -7.563  1.00 24.22  A C
ATOM 1071  CG  ASP A 170    -9.203  41.517  -8.606  1.00 24.66  A C
ATOM 1072  OD1 ASP A 170    -9.267  40.310  -8.285  1.00 24.57  A O
ATOM 1073  OD2 ASP A 170    -8.911  41.889  -9.761  1.00 25.02  A O
ATOM 1074  C   ASP A 170   -10.815  41.243  -5.913  1.00 24.39  A C
ATOM 1075  O   ASP A 170   -11.824  41.804  -5.504  1.00 24.45  A O
ATOM 1076  N   GLU A 171   -10.768  39.941  -6.186  1.00 24.63  A N
ATOM 1077  CA  GLU A 171   -11.929  39.070  -6.022  1.00 25.10  A C
ATOM 1078  CB  GLU A 171   -11.649  37.680  -6.582  1.00 26.33  A C
ATOM 1079  CG  GLU A 171   -11.608  37.592  -8.087  1.00 28.10  A C
ATOM 1080  CD  GLU A 171   -11.209  36.212  -8.544  1.00 29.44  A C
ATOM 1081  OE1 GLU A 171   -10.098  35.777  -8.202  1.00 30.78  A O
ATOM 1082  OE2 GLU A 171   -12.001  35.546  -9.239  1.00 30.62  A O
ATOM 1083  C   GLU A 171   -12.354  38.897  -4.576  1.00 24.83  A C
ATOM 1084  O   GLU A 171   -13.481  38.473  -4.309  1.00 24.83  A O
ATOM 1085  N   ASN A 172   -11.445  39.192  -3.649  1.00 24.23  A N
ATOM 1086  CA  ASN A 172   -11.739  39.055  -2.233  1.00 23.92  A C
ATOM 1087  CB  ASN A 172   -10.660  38.221  -1.538  1.00 23.71  A C
ATOM 1088  CG  ASN A 172   -10.676  36.796  -2.003  1.00 23.57  A C
ATOM 1089  OD1 ASN A 172   -11.746  36.277  -2.336  1.00 23.91  A O
ATOM 1090  ND2 ASN A 172    -9.510  36.143  -2.034  1.00 23.03  A N
ATOM 1091  C   ASN A 172   -11.896  40.377  -1.528  1.00 23.72  A C
ATOM 1092  O   ASN A 172   -11.675  40.465  -0.320  1.00 23.71  A O
ATOM 1093  N   ILE A 173   -12.266  41.402  -2.294  1.00 23.46  A N
ATOM 1094  CA  ILE A 173   -12.491  42.733  -1.757  1.00 23.41  A C
ATOM 1095  CB  ILE A 173   -11.414  43.719  -2.247  1.00 23.08  A C
ATOM 1096  CG2 ILE A 173   -11.792  45.139  -1.864  1.00 22.39  A C
ATOM 1097  CG1 ILE A 173   -10.057  43.336  -1.654  1.00 22.89  A C
ATOM 1098  CD1 ILE A 173    -8.882  44.082  -2.257  1.00 22.07  A C
ATOM 1099  C   ILE A 173   -13.878  43.239  -2.192  1.00 23.82  A C
ATOM 1100  O   ILE A 173   -14.187  43.320  -3.386  1.00 23.90  A O
ATOM 1101  N   LEU A 174   -14.715  43.556  -1.212  1.00 24.24  A N
ATOM 1102  CA  LEU A 174   -16.058  44.065  -1.471  1.00 24.64  A C
ATOM 1103  CB  LEU A 174   -17.035  43.509  -0.440  1.00 24.77  A C
ATOM 1104  CG  LEU A 174   -17.855  42.269  -0.793  1.00 25.22  A C
ATOM 1105  CD1 LEU A 174   -17.107  41.381  -1.780  1.00 24.66  A C
ATOM 1106  CD2 LEU A 174   -18.215  41.540   0.488  1.00 24.62  A C
ATOM 1107  C   LEU A 174   -16.059  45.581  -1.369  1.00 24.89  A C
ATOM 1108  O   LEU A 174   -15.370  46.154  -0.509  1.00 24.41  A O
ATOM 1109  N   ILE A 175   -16.816  46.229  -2.250  1.00 25.04  A N
ATOM 1110  CA  ILE A 175   -16.935  47.684  -2.206  1.00 25.60  A C
ATOM 1111  CB  ILE A 175   -16.651  48.355  -3.579  1.00 25.15  A C
ATOM 1112  CG2 ILE A 175   -16.826  49.866  -3.471  1.00 24.78  A C
ATOM 1113  CG1 ILE A 175   -15.243  48.050  -4.061  1.00 24.53  A C
ATOM 1114  CD1 ILE A 175   -15.080  48.402  -5.499  1.00 23.83  A C
ATOM 1115  C   ILE A 175   -18.366  48.090  -1.834  1.00 26.42  A C
ATOM 1116  O   ILE A 175   -19.311  47.756  -2.548  1.00 26.56  A O
ATOM 1117  N   ASP A 176   -18.533  48.792  -0.715  1.00 27.26  A N
ATOM 1118  CA  ASP A 176   -19.850  49.300  -0.355  1.00 28.12  A C
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FIGURE 2A-21

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ATOM 1119  CB  ASP A 176  -19.902  49.627   1.139  1.00 28.61  A C
ATOM 1120  CG  ASP A 176  -21.196  50.313   1.546  1.00 29.25  A C
ATOM 1121  OD1 ASP A 176  -21.517  50.308   2.755  1.00 29.11  A O
ATOM 1122  OD2 ASP A 176  -21.882  50.872   0.656  1.00 29.67  A O
ATOM 1123  C   ASP A 176  -19.930  50.578  -1.216  1.00 28.68  A C
ATOM 1124  O   ASP A 176  -19.284  51.592  -0.921  1.00 28.54  A O
ATOM 1125  N   LEU A 177  -20.689  50.495  -2.306  1.00 29.26  A N
ATOM 1126  CA  LEU A 177  -20.843  51.596  -3.256  1.00 30.07  A C
ATOM 1127  CB  LEU A 177  -21.668  51.117  -4.452  1.00 29.99  A C
ATOM 1128  CG  LEU A 177  -21.013  49.980  -5.251  1.00 30.29  A C
ATOM 1129  CD1 LEU A 177  -22.023  49.412  -6.256  1.00 30.03  A C
ATOM 1130  CD2 LEU A 177  -19.744  50.490  -5.953  1.00 29.15  A C
ATOM 1131  C   LEU A 177  -21.423  52.912  -2.731  1.00 30.74  A C
ATOM 1132  O   LEU A 177  -21.175  53.964  -3.321  1.00 31.10  A O
ATOM 1133  N   ASN A 178  -22.186  52.877  -1.640  1.00 31.31  A N
ATOM 1134  CA  ASN A 178  -22.751  54.112  -1.096  1.00 32.02  A C
ATOM 1135  CB  ASN A 178  -24.139  53.855  -0.487  1.00 32.79  A C
ATOM 1136  CG  ASN A 178  -25.212  53.606  -1.550  1.00 34.17  A C
ATOM 1137  OD1 ASN A 178  -26.338  53.210  -1.225  1.00 35.14  A O
ATOM 1138  ND2 ASN A 178  -24.873  53.845  -2.825  1.00 34.30  A N
ATOM 1139  C   ASN A 178  -21.847  54.788  -0.058  1.00 31.94  A C
ATOM 1140  O   ASN A 178  -21.724  56.015  -0.051  1.00 31.88  A O
ATOM 1141  N   ARG A 179  -21.205  53.997   0.802  1.00 31.86  A N
ATOM 1142  CA  ARG A 179  -20.322  54.558   1.829  1.00 31.75  A C
ATOM 1143  CB  ARG A 179  -20.428  53.732   3.118  1.00 32.63  A C
ATOM 1144  CG  ARG A 179  -21.823  53.182   3.355  1.00 33.83  A C
ATOM 1145  CD  ARG A 179  -22.181  53.089   4.822  1.00 34.88  A C
ATOM 1146  NE  ARG A 179  -22.184  54.421   5.405  1.00 36.30  A N
ATOM 1147  CZ  ARG A 179  -23.036  54.836   6.339  1.00 36.94  A C
ATOM 1148  NH1 ARG A 179  -23.973  54.022   6.809  1.00 37.37  A N
ATOM 1149  NH2 ARG A 179  -22.951  56.077   6.801  1.00 37.27  A N
ATOM 1150  C   ARG A 179  -18.854  54.645   1.386  1.00 31.29  A C
ATOM 1151  O   ARG A 179  -18.034  55.297   2.043  1.00 31.07  A O
ATOM 1152  N   GLY A 180  -18.530  54.001   0.263  1.00 30.77  A N
ATOM 1153  CA  GLY A 180  -17.165  54.021  -0.243  1.00 30.01  A C
ATOM 1154  C   GLY A 180  -16.180  53.234   0.616  1.00 29.59  A C
ATOM 1155  O   GLY A 180  -14.992  53.562   0.648  1.00 29.54  A O
ATOM 1156  N   GLU A 181  -16.663  52.195   1.296  1.00 28.70  A N
ATOM 1157  CA  GLU A 181  -15.816  51.379   2.168  1.00 28.23  A C
ATOM 1158  CB  GLU A 181  -16.490  51.203   3.537  1.00 28.40  A C
ATOM 1159  CG  GLU A 181  -16.910  52.533   4.145  1.00 29.31  A C
ATOM 1160  CD  GLU A 181  -17.706  52.420   5.437  1.00 29.31  A C
ATOM 1161  OE1 GLU A 181  -18.210  51.331   5.762  1.00 29.98  A O
ATOM 1162  OE2 GLU A 181  -17.848  53.449   6.127  1.00 29.79  A O
ATOM 1163  C   GLU A 181  -15.521  50.009   1.574  1.00 27.60  A C
ATOM 1164  O   GLU A 181  -16.409  49.377   0.997  1.00 27.21  A O
ATOM 1165  N   LEU A 182  -14.268  49.561   1.704  1.00 26.81  A N
ATOM 1166  CA  LEU A 182  -13.891  48.247   1.202  1.00 26.15  A C
ATOM 1167  CB  LEU A 182  -12.516  48.274   0.514  1.00 25.73  A C
ATOM 1168  CG  LEU A 182  -12.230  49.250  -0.641  1.00 26.23  A C
ATOM 1169  CD1 LEU A 182  -11.150  48.655  -1.555  1.00 25.40  A C
ATOM 1170  CD2 LEU A 182  -13.470  49.531  -1.437  1.00 25.65  A C
ATOM 1171  C   LEU A 182  -13.877  47.250   2.364  1.00 25.73  A C
ATOM 1172  O   LEU A 182  -13.591  47.612   3.505  1.00 25.26  A O
ATOM 1173  N   LYS A 183  -14.202  45.995   2.066  1.00 25.60  A N
ATOM 1174  CA  LYS A 183  -14.231  44.936   3.078  1.00 25.63  A C
```

FIGURE 2A-22

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ATOM 1175  CB  LYS A 183  -15.669  44.548   3.416  1.00 26.14  A C
ATOM 1176  CG  LYS A 183  -16.574  45.687   3.812  1.00 27.11  A C
ATOM 1177  CD  LYS A 183  -16.336  46.098   5.235  1.00 27.92  A C
ATOM 1178  CE  LYS A 183  -17.516  46.882   5.768  1.00 28.38  A C
ATOM 1179  NZ  LYS A 183  -17.219  47.277   7.173  1.00 29.66  A N
ATOM 1180  C   LYS A 183  -13.518  43.699   2.544  1.00 25.27  A C
ATOM 1181  O   LYS A 183  -13.714  43.313   1.396  1.00 25.00  A O
ATOM 1182  N   LEU A 184  -12.712  43.073   3.388  1.00 25.19  A N
ATOM 1183  CA  LEU A 184  -11.967  41.876   3.017  1.00 25.40  A C
ATOM 1184  CB  LEU A 184  -10.695  41.790   3.858  1.00 26.03  A C
ATOM 1185  CG  LEU A 184   -9.342  41.805   3.153  1.00 27.30  A C
ATOM 1186  CD1 LEU A 184   -9.228  40.583   2.255  1.00 27.60  A C
ATOM 1187  CD2 LEU A 184   -9.184  43.092   2.327  1.00 27.66  A C
ATOM 1188  C   LEU A 184  -12.814  40.608   3.243  1.00 25.12  A C
ATOM 1189  O   LEU A 184  -13.433  40.446   4.295  1.00 24.62  A O
ATOM 1190  N   ILE A 185  -12.830  39.708   2.263  1.00 24.77  A N
ATOM 1191  CA  ILE A 185  -13.593  38.480   2.409  1.00 24.64  A C
ATOM 1192  CB  ILE A 185  -14.814  38.430   1.469  1.00 24.43  A C
ATOM 1193  CG2 ILE A 185  -15.838  39.496   1.869  1.00 24.08  A C
ATOM 1194  CG1 ILE A 185  -14.339  38.556   0.019  1.00 23.87  A C
ATOM 1195  CD1 ILE A 185  -15.427  38.429  -0.980  1.00 23.55  A C
ATOM 1196  C   ILE A 185  -12.753  37.261   2.086  1.00 24.95  A C
ATOM 1197  O   ILE A 185  -11.679  37.363   1.488  1.00 24.98  A O
ATOM 1198  N   ASP A 186  -13.277  36.110   2.490  1.00 25.30  A N
ATOM 1199  CA  ASP A 186  -12.665  34.813   2.271  1.00 25.60  A C
ATOM 1200  CB  ASP A 186  -12.505  34.532   0.776  1.00 25.82  A C
ATOM 1201  CG  ASP A 186  -12.151  33.071   0.500  1.00 26.48  A C
ATOM 1202  OD1 ASP A 186  -12.348  32.244   1.419  1.00 26.81  A O
ATOM 1203  OD2 ASP A 186  -11.698  32.742  -0.624  1.00 26.64  A O
ATOM 1204  C   ASP A 186  -11.338  34.557   2.970  1.00 25.92  A C
ATOM 1205  O   ASP A 186  -10.252  34.773   2.409  1.00 25.67  A O
ATOM 1206  N   PHE A 187  -11.436  34.065   4.198  1.00 26.16  A N
ATOM 1207  CA  PHE A 187  -10.252  33.720   4.963  1.00 26.58  A C
ATOM 1208  CB  PHE A 187  -10.422  34.145   6.414  1.00 26.34  A C
ATOM 1209  CG  PHE A 187  -10.247  35.615   6.623  1.00 26.11  A C
ATOM 1210  CD1 PHE A 187  -11.187  36.519   6.138  1.00 26.12  A C
ATOM 1211  CD2 PHE A 187   -9.112  36.102   7.257  1.00 25.65  A C
ATOM 1212  CE1 PHE A 187  -10.991  37.898   6.279  1.00 26.11  A C
ATOM 1213  CE2 PHE A 187   -8.910  37.463   7.403  1.00 25.71  A C
ATOM 1214  CZ  PHE A 187   -9.847  38.367   6.913  1.00 25.92  A C
ATOM 1215  C   PHE A 187   -9.993  32.227   4.890  1.00 26.86  A C
ATOM 1216  O   PHE A 187   -9.288  31.668   5.726  1.00 27.56  A O
ATOM 1217  N   GLY A 188  -10.536  31.589   3.863  1.00 27.02  A N
ATOM 1218  CA  GLY A 188  -10.383  30.151   3.714  1.00 27.29  A C
ATOM 1219  C   GLY A 188   -9.004  29.597   3.418  1.00 27.40  A C
ATOM 1220  O   GLY A 188   -8.809  28.387   3.479  1.00 27.56  A O
ATOM 1221  N   SER A 189   -8.049  30.453   3.074  1.00 27.51  A N
ATOM 1222  CA  SER A 189   -6.691  29.991   2.802  1.00 27.44  A C
ATOM 1223  CB  SER A 189   -6.234  30.441   1.414  1.00 27.86  A C
ATOM 1224  OG  SER A 189   -7.155  30.066   0.398  1.00 28.90  A O
ATOM 1225  C   SER A 189   -5.767  30.609   3.842  1.00 27.22  A C
ATOM 1226  O   SER A 189   -4.545  30.482   3.752  1.00 27.37  A O
ATOM 1227  N   GLY A 190   -6.360  31.287   4.819  1.00 26.86  A N
ATOM 1228  CA  GLY A 190   -5.576  31.963   5.836  1.00 26.90  A C
ATOM 1229  C   GLY A 190   -4.891  31.073   6.852  1.00 27.00  A C
ATOM 1230  O   GLY A 190   -4.921  29.841   6.756  1.00 27.23  A O
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FIGURE 2A-23

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ATOM 1231  N   ALA A 191   -4.267  31.698   7.841  1.00 26.68  A N
ATOM 1232  CA  ALA A 191   -3.566  30.953   8.875  1.00 26.62  A C
ATOM 1233  CB  ALA A 191   -2.235  30.423   8.337  1.00 26.29  A C
ATOM 1234  C   ALA A 191   -3.305  31.885  10.022  1.00 26.66  A C
ATOM 1235  O   ALA A 191   -3.453  33.100   9.886  1.00 26.69  A O
ATOM 1236  N   LEU A 192   -2.931  31.322  11.163  1.00 26.77  A N
ATOM 1237  CA  LEU A 192   -2.603  32.149  12.297  1.00 26.99  A C
ATOM 1238  CB  LEU A 192   -2.411  31.287  13.541  1.00 27.51  A C
ATOM 1239  CG  LEU A 192   -3.706  30.600  13.983  1.00 28.39  A C
ATOM 1240  CD1 LEU A 192   -3.416  29.509  15.018  1.00 28.76  A C
ATOM 1241  CD2 LEU A 192   -4.651  31.664  14.551  1.00 28.47  A C
ATOM 1242  C   LEU A 192   -1.287  32.767  11.858  1.00 26.85  A C
ATOM 1243  O   LEU A 192   -0.490  32.112  11.184  1.00 26.76  A O
ATOM 1244  N   LEU A 193   -1.073  34.031  12.189  1.00 26.72  A N
ATOM 1245  CA  LEU A 193    0.165  34.699  11.822  1.00 26.89  A C
ATOM 1246  CB  LEU A 193    0.013  36.215  11.985  1.00 26.83  A C
ATOM 1247  CG  LEU A 193    1.224  37.102  11.659  1.00 26.55  A C
ATOM 1248  CD1 LEU A 193    1.522  37.049  10.175  1.00 26.12  A C
ATOM 1249  CD2 LEU A 193    0.937  38.540  12.092  1.00 26.36  A C
ATOM 1250  C   LEU A 193    1.264  34.177  12.749  1.00 27.26  A C
ATOM 1251  O   LEU A 193    1.015  33.901  13.924  1.00 27.02  A O
ATOM 1252  N   LYS A 194    2.470  34.034  12.206  1.00 27.62  A N
ATOM 1253  CA  LYS A 194    3.618  33.550  12.958  1.00 28.03  A C
ATOM 1254  CB  LYS A 194    3.719  32.019  12.863  1.00 27.97  A C
ATOM 1255  CG  LYS A 194    3.995  31.497  11.461  1.00 28.29  A C
ATOM 1256  CD  LYS A 194    4.050  29.978  11.436  1.00 28.43  A C
ATOM 1257  CE  LYS A 194    4.348  29.485  10.019  1.00 28.62  A C
ATOM 1258  NZ  LYS A 194    4.405  27.993   9.922  1.00 28.98  A N
ATOM 1259  C   LYS A 194    4.854  34.196  12.349  1.00 28.21  A C
ATOM 1260  O   LYS A 194    4.784  34.730  11.237  1.00 28.30  A O
ATOM 1261  N   ASP A 195    5.978  34.146  13.067  1.00 28.55  A N
ATOM 1262  CA  ASP A 195    7.227  34.745  12.589  1.00 28.83  A C
ATOM 1263  CB  ASP A 195    7.972  35.403  13.753  1.00 28.94  A C
ATOM 1264  CG  ASP A 195    7.156  36.501  14.411  1.00 29.24  A C
ATOM 1265  OD1 ASP A 195    6.877  36.409  15.625  1.00 29.48  A O
ATOM 1266  OD2 ASP A 195    6.780  37.463  13.709  1.00 29.73  A O
ATOM 1267  C   ASP A 195    8.133  33.738  11.884  1.00 29.01  A C
ATOM 1268  O   ASP A 195    9.121  34.120  11.253  1.00 29.03  A O
ATOM 1269  N   THR A 196    7.785  32.458  11.982  1.00 28.98  A N
ATOM 1270  CA  THR A 196    8.548  31.394  11.333  1.00 29.17  A C
ATOM 1271  CB  THR A 196    8.425  30.076  12.119  1.00 29.10  A C
ATOM 1272  OG1 THR A 196    7.047  29.826  12.418  1.00 29.14  A O
ATOM 1273  CG2 THR A 196    9.215  30.155  13.429  1.00 29.14  A C
ATOM 1274  C   THR A 196    8.060  31.176   9.893  1.00 29.44  A C
ATOM 1275  O   THR A 196    7.008  31.698   9.492  1.00 29.59  A O
ATOM 1276  N   VAL A 197    8.811  30.386   9.130  1.00 29.46  A N
ATOM 1277  CA  VAL A 197    8.509  30.126   7.724  1.00 29.50  A C
ATOM 1278  CB  VAL A 197    9.722  29.452   7.029  1.00 29.43  A C
ATOM 1279  CG1 VAL A 197    9.906  28.016   7.548  1.00 29.43  A C
ATOM 1280  CG2 VAL A 197    9.529  29.462   5.513  1.00 29.43  A C
ATOM 1281  C   VAL A 197    7.250  29.299   7.444  1.00 29.57  A C
ATOM 1282  O   VAL A 197    6.877  28.431   8.219  1.00 30.06  A O
ATOM 1283  N   TYR A 198    6.588  29.601   6.333  1.00 29.70  A N
ATOM 1284  CA  TYR A 198    5.387  28.881   5.902  1.00 29.70  A C
ATOM 1285  CB  TYR A 198    4.299  29.856   5.412  1.00 28.46  A C
ATOM 1286  CG  TYR A 198    3.576  30.631   6.494  1.00 27.20  A C
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FIGURE 2A-24

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ATOM 1287  CD1 TYR A 198     2.447  30.101   7.120  1.00 26.71  A C
ATOM 1288  CE1 TYR A 198     1.752  30.816   8.098  1.00 26.00  A C
ATOM 1289  CD2 TYR A 198     4.004  31.906   6.875  1.00 26.46  A C
ATOM 1290  CE2 TYR A 198     3.321  32.629   7.850  1.00 26.06  A C
ATOM 1291  CZ  TYR A 198     2.189  32.076   8.457  1.00 26.08  A C
ATOM 1292  OH  TYR A 198     1.479  32.786   9.401  1.00 25.24  A O
ATOM 1293  C   TYR A 198     5.822  28.008   4.726  1.00 30.38  A C
ATOM 1294  O   TYR A 198     6.531  28.473   3.830  1.00 30.51  A O
ATOM 1295  N   THR A 199     5.399  26.750   4.726  1.00 31.31  A N
ATOM 1296  CA  THR A 199     5.747  25.832   3.651  1.00 32.20  A C
ATOM 1297  CB  THR A 199     6.479  24.610   4.198  1.00 32.48  A C
ATOM 1298  OG1 THR A 199     5.698  24.039   5.252  1.00 32.75  A O
ATOM 1299  CG2 THR A 199     7.837  25.012   4.744  1.00 32.63  A C
ATOM 1300  C   THR A 199     4.487  25.367   2.950  1.00 32.68  A C
ATOM 1301  O   THR A 199     4.540  24.535   2.044  1.00 32.83  A O
ATOM 1302  N   ASP A 200     3.349  25.901   3.384  1.00 33.37  A N
ATOM 1303  CA  ASP A 200     2.062  25.563   2.779  1.00 34.01  A C
ATOM 1304  CB  ASP A 200     1.104  24.971   3.817  1.00 34.59  A C
ATOM 1305  CG  ASP A 200     0.554  26.024   4.774  1.00 35.51  A C
ATOM 1306  OD1 ASP A 200     1.366  26.665   5.475  1.00 35.77  A O
ATOM 1307  OD2 ASP A 200    -0.685  26.211   4.829  1.00 35.95  A O
ATOM 1308  C   ASP A 200     1.437  26.827   2.197  1.00 34.03  A C
ATOM 1309  O   ASP A 200     1.568  27.912   2.766  1.00 33.96  A O
ATOM 1310  N   PHE A 201     0.774  26.679   1.055  1.00 33.88  A N
ATOM 1311  CA  PHE A 201     0.104  27.791   0.403  1.00 33.84  A C
ATOM 1312  CB  PHE A 201     1.089  28.637  -0.397  1.00 33.43  A C
ATOM 1313  CG  PHE A 201     0.439  29.783  -1.141  1.00 33.14  A C
ATOM 1314  CD1 PHE A 201     0.295  29.745  -2.525  1.00 33.02  A C
ATOM 1315  CD2 PHE A 201    -0.034  30.897  -0.451  1.00 32.97  A C
ATOM 1316  CE1 PHE A 201    -0.310  30.800  -3.214  1.00 33.37  A C
ATOM 1317  CE2 PHE A 201    -0.641  31.956  -1.123  1.00 33.22  A C
ATOM 1318  CZ  PHE A 201    -0.781  31.914  -2.508  1.00 33.44  A C
ATOM 1319  C   PHE A 201    -0.979  27.283  -0.533  1.00 34.14  A C
ATOM 1320  O   PHE A 201    -0.741  26.391  -1.330  1.00 34.51  A O
ATOM 1321  N   ASP A 202    -2.171  27.850  -0.435  1.00 34.43  A N
ATOM 1322  CA  ASP A 202    -3.251  27.443  -1.308  1.00 34.78  A C
ATOM 1323  CB  ASP A 202    -4.184  26.451  -0.593  1.00 35.64  A C
ATOM 1324  CG  ASP A 202    -5.264  25.892  -1.522  1.00 36.39  A C
ATOM 1325  OD1 ASP A 202    -4.918  25.404  -2.621  1.00 36.72  A O
ATOM 1326  OD2 ASP A 202    -6.459  25.942  -1.156  1.00 36.92  A O
ATOM 1327  C   ASP A 202    -4.024  28.669  -1.780  1.00 34.57  A C
ATOM 1328  O   ASP A 202    -5.203  28.582  -2.119  1.00 34.70  A O
ATOM 1329  N   GLY A 203    -3.352  29.814  -1.810  1.00 34.12  A N
ATOM 1330  CA  GLY A 203    -4.006  31.028  -2.266  1.00 33.44  A C
ATOM 1331  C   GLY A 203    -3.955  31.113  -3.778  1.00 32.86  A C
ATOM 1332  O   GLY A 203    -3.810  30.100  -4.444  1.00 33.00  A O
ATOM 1333  N   THR A 204    -4.064  32.316  -4.326  1.00 32.36  A N
ATOM 1334  CA  THR A 204    -4.032  32.495  -5.771  1.00 31.79  A C
ATOM 1335  CB  THR A 204    -4.807  33.751  -6.173  1.00 31.69  A C
ATOM 1336  OG1 THR A 204    -6.141  33.656  -5.654  1.00 31.30  A O
ATOM 1337  CG2 THR A 204    -4.854  33.889  -7.699  1.00 31.39  A C
ATOM 1338  C   THR A 204    -2.590  32.606  -6.246  1.00 31.57  A C
ATOM 1339  O   THR A 204    -1.852  33.493  -5.811  1.00 31.64  A O
ATOM 1340  N   ARG A 205    -2.199  31.722  -7.157  1.00 31.12  A N
ATOM 1341  CA  ARG A 205    -0.826  31.687  -7.635  1.00 31.00  A C
ATOM 1342  CB  ARG A 205    -0.636  30.506  -8.602  1.00 31.60  A C
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FIGURE 2A-25

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ATOM 1343  CG  ARG A 205     0.825  30.044  -8.716  1.00 32.44  A C
ATOM 1344  CD  ARG A 205     0.988  28.873  -9.679  1.00 32.79  A C
ATOM 1345  NE  ARG A 205     2.388  28.479  -9.867  1.00 33.35  A N
ATOM 1346  CZ  ARG A 205     3.131  27.821  -8.974  1.00 33.54  A C
ATOM 1347  NH1 ARG A 205     2.629  27.467  -7.796  1.00 33.59  A N
ATOM 1348  NH2 ARG A 205     4.381  27.493  -9.271  1.00 33.29  A N
ATOM 1349  C   ARG A 205    -0.250  32.974  -8.250  1.00 30.49  A C
ATOM 1350  O   ARG A 205     0.847  33.396  -7.867  1.00 30.40  A O
ATOM 1351  N   VAL A 206    -0.964  33.603  -9.183  1.00 29.68  A N
ATOM 1352  CA  VAL A 206    -0.453  34.825  -9.807  1.00 28.80  A C
ATOM 1353  CB  VAL A 206    -1.357  35.310 -10.987  1.00 29.01  A C
ATOM 1354  CG1 VAL A 206    -1.281  34.314 -12.144  1.00 28.69  A C
ATOM 1355  CG2 VAL A 206    -2.810  35.486 -10.526  1.00 28.52  A C
ATOM 1356  C   VAL A 206    -0.274  35.960  -8.793  1.00 28.47  A C
ATOM 1357  O   VAL A 206     0.239  37.022  -9.139  1.00 28.31  A O
ATOM 1358  N   TYR A 207    -0.711  35.734  -7.550  1.00 28.00  A N
ATOM 1359  CA  TYR A 207    -0.554  36.717  -6.466  1.00 27.56  A C
ATOM 1360  CB  TYR A 207    -1.872  36.952  -5.709  1.00 27.64  A C
ATOM 1361  CG  TYR A 207    -2.832  37.937  -6.351  1.00 27.74  A C
ATOM 1362  CD1 TYR A 207    -3.679  37.553  -7.394  1.00 27.49  A C
ATOM 1363  CE1 TYR A 207    -4.540  38.461  -7.990  1.00 27.71  A C
ATOM 1364  CD2 TYR A 207    -2.874  39.261  -5.920  1.00 27.63  A C
ATOM 1365  CE2 TYR A 207    -3.728  40.175  -6.501  1.00 27.78  A C
ATOM 1366  CZ  TYR A 207    -4.558  39.772  -7.535  1.00 28.00  A C
ATOM 1367  OH  TYR A 207    -5.399  40.701  -8.100  1.00 28.64  A O
ATOM 1368  C   TYR A 207     0.490  36.239  -5.445  1.00 27.20  A C
ATOM 1369  O   TYR A 207     0.760  36.941  -4.461  1.00 26.90  A O
ATOM 1370  N   SER A 208     1.045  35.040  -5.666  1.00 26.65  A N
ATOM 1371  CA  SER A 208     2.047  34.458  -4.765  1.00 26.59  A C
ATOM 1372  CB  SER A 208     2.019  32.918  -4.829  1.00 26.62  A C
ATOM 1373  OG  SER A 208     2.493  32.434  -6.074  1.00 26.37  A O
ATOM 1374  C   SER A 208     3.438  34.970  -5.127  1.00 26.58  A C
ATOM 1375  O   SER A 208     3.734  35.186  -6.304  1.00 26.75  A O
ATOM 1376  N   PRO A 209     4.317  35.134  -4.123  1.00 26.45  A N
ATOM 1377  CD  PRO A 209     4.056  34.765  -2.719  1.00 26.39  A C
ATOM 1378  CA  PRO A 209     5.689  35.632  -4.289  1.00 26.44  A C
ATOM 1379  CB  PRO A 209     6.080  36.006  -2.862  1.00 26.39  A C
ATOM 1380  CG  PRO A 209     5.421  34.906  -2.061  1.00 26.41  A C
ATOM 1381  C   PRO A 209     6.704  34.685  -4.933  1.00 26.67  A C
ATOM 1382  O   PRO A 209     6.528  33.466  -4.942  1.00 26.62  A O
ATOM 1383  N   PRO A 210     7.803  35.249  -5.468  1.00 26.89  A N
ATOM 1384  CD  PRO A 210     8.196  36.664  -5.349  1.00 26.95  A C
ATOM 1385  CA  PRO A 210     8.865  34.469  -6.117  1.00 26.93  A C
ATOM 1386  CB  PRO A 210     9.940  35.513  -6.432  1.00 26.80  A C
ATOM 1387  CG  PRO A 210     9.227  36.796  -6.431  1.00 27.26  A C
ATOM 1388  C   PRO A 210     9.433  33.377  -5.206  1.00 27.10  A C
ATOM 1389  O   PRO A 210     9.798  32.304  -5.690  1.00 27.00  A O
ATOM 1390  N   GLU A 211     9.529  33.668  -3.904  1.00 27.30  A N
ATOM 1391  CA  GLU A 211    10.078  32.711  -2.937  1.00 27.78  A C
ATOM 1392  CB  GLU A 211    10.343  33.364  -1.563  1.00 26.90  A C
ATOM 1393  CG  GLU A 211     9.130  34.001  -0.907  1.00 26.71  A C
ATOM 1394  CD  GLU A 211     8.943  35.475  -1.279  1.00 26.25  A C
ATOM 1395  OE1 GLU A 211     9.382  35.897  -2.376  1.00 25.69  A O
ATOM 1396  OE2 GLU A 211     8.336  36.201  -0.468  1.00 25.74  A O
ATOM 1397  C   GLU A 211     9.172  31.498  -2.781  1.00 28.33  A C
ATOM 1398  O   GLU A 211     9.660  30.397  -2.532  1.00 28.53  A O
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FIGURE 2A-26

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ATOM 1399  N   TRP A 212     7.860  31.675  -2.911  1.00 28.92  A N
ATOM 1400  CA  TRP A 212     6.985  30.509  -2.830  1.00 29.60  A C
ATOM 1401  CB  TRP A 212     5.515  30.906  -2.693  1.00 29.49  A C
ATOM 1402  CG  TRP A 212     4.583  29.768  -3.022  1.00 29.33  A C
ATOM 1403  CD2 TRP A 212     4.369  28.577  -2.249  1.00 29.28  A C
ATOM 1404  CE2 TRP A 212     3.457  27.766  -2.972  1.00 29.36  A C
ATOM 1405  CE3 TRP A 212     4.859  28.115  -1.017  1.00 29.26  A C
ATOM 1406  CD1 TRP A 212     3.820  29.636  -4.143  1.00 29.41  A C
ATOM 1407  NE1 TRP A 212     3.136  28.437  -4.122  1.00 29.58  A N
ATOM 1408  CZ2 TRP A 212     3.026  26.517  -2.504  1.00 29.00  A C
ATOM 1409  CZ3 TRP A 212     4.424  26.865  -0.550  1.00 29.11  A C
ATOM 1410  CH2 TRP A 212     3.516  26.085  -1.299  1.00 29.20  A C
ATOM 1411  C   TRP A 212     7.155  29.675  -4.110  1.00 30.34  A C
ATOM 1412  O   TRP A 212     7.253  28.447  -4.050  1.00 30.63  A O
ATOM 1413  N   ILE A 213     7.192  30.350  -5.261  1.00 31.07  A N
ATOM 1414  CA  ILE A 213     7.345  29.678  -6.554  1.00 31.91  A C
ATOM 1415  CB  ILE A 213     7.394  30.697  -7.725  1.00 31.71  A C
ATOM 1416  CG2 ILE A 213     7.481  29.957  -9.051  1.00 31.88  A C
ATOM 1417  CG1 ILE A 213     6.162  31.604  -7.722  1.00 31.73  A C
ATOM 1418  CD1 ILE A 213     4.873  30.931  -8.109  1.00 31.95  A C
ATOM 1419  C   ILE A 213     8.630  28.829  -6.626  1.00 32.67  A C
ATOM 1420  O   ILE A 213     8.596  27.668  -7.027  1.00 32.77  A O
ATOM 1421  N   ARG A 214     9.755  29.410  -6.218  1.00 33.55  A N
ATOM 1422  CA  ARG A 214    11.055  28.737  -6.277  1.00 34.24  A C
ATOM 1423  CB  ARG A 214    12.177  29.773  -6.354  1.00 35.12  A C
ATOM 1424  CG  ARG A 214    12.044  30.797  -7.455  1.00 36.90  A C
ATOM 1425  CD  ARG A 214    13.166  31.817  -7.352  1.00 38.19  A C
ATOM 1426  NE  ARG A 214    14.464  31.213  -7.637  1.00 40.06  A N
ATOM 1427  CZ  ARG A 214    15.639  31.755  -7.309  1.00 40.87  A C
ATOM 1428  NH1 ARG A 214    15.689  32.923  -6.677  1.00 41.10  A N
ATOM 1429  NH2 ARG A 214    16.772  31.125  -7.613  1.00 41.19  A N
ATOM 1430  C   ARG A 214    11.419  27.779  -5.148  1.00 34.32  A C
ATOM 1431  O   ARG A 214    12.094  26.788  -5.390  1.00 34.37  A O
ATOM 1432  N   TYR A 215    10.990  28.067  -3.922  1.00 34.42  A N
ATOM 1433  CA  TYR A 215    11.366  27.233  -2.782  1.00 34.25  A C
ATOM 1434  CB  TYR A 215    12.304  28.014  -1.873  1.00 34.94  A C
ATOM 1435  CG  TYR A 215    13.384  28.740  -2.612  1.00 35.73  A C
ATOM 1436  CD1 TYR A 215    14.349  28.038  -3.341  1.00 36.29  A C
ATOM 1437  CE1 TYR A 215    15.356  28.711  -4.036  1.00 36.71  A C
ATOM 1438  CD2 TYR A 215    13.447  30.133  -2.593  1.00 36.01  A C
ATOM 1439  CE2 TYR A 215    14.447  30.817  -3.286  1.00 36.56  A C
ATOM 1440  CZ  TYR A 215    15.395  30.099  -4.002  1.00 36.93  A C
ATOM 1441  OH  TYR A 215    16.382  30.773  -4.686  1.00 38.16  A O
ATOM 1442  C   TYR A 215    10.242  26.736  -1.919  1.00 33.88  A C
ATOM 1443  O   TYR A 215    10.484  26.049  -0.931  1.00 33.85  A O
ATOM 1444  N   HIS A 216     9.016  27.088  -2.268  1.00 33.44  A N
ATOM 1445  CA  HIS A 216     7.886  26.694  -1.450  1.00 33.09  A C
ATOM 1446  CB  HIS A 216     7.646  25.185  -1.538  1.00 33.56  A C
ATOM 1447  CG  HIS A 216     6.808  24.792  -2.716  1.00 34.88  A C
ATOM 1448  CD2 HIS A 216     6.589  25.416  -3.900  1.00 35.15  A C
ATOM 1449  ND1 HIS A 216     6.050  23.639  -2.748  1.00 35.35  A N
ATOM 1450  CE1 HIS A 216     5.402  23.572  -3.898  1.00 35.35  A C
ATOM 1451  NE2 HIS A 216     5.712  24.638  -4.615  1.00 35.49  A N
ATOM 1452  C   HIS A 216     8.088  27.128  -0.002  1.00 32.37  A C
ATOM 1453  O   HIS A 216     7.748  26.407   0.922  1.00 32.60  A O
ATOM 1454  N   ARG A 217     8.652  28.317   0.182  1.00 31.57  A N
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FIGURE 2A-27

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ATOM 1455  CA  ARG A 217     8.889  28.880   1.518  1.00 30.76  A C
ATOM 1456  CB  ARG A 217    10.343  28.648   1.973  1.00 30.71  A C
ATOM 1457  CG  ARG A 217    10.766  27.200   2.189  1.00 30.70  A C
ATOM 1458  CD  ARG A 217    12.302  27.099   2.300  1.00 30.60  A C
ATOM 1459  NE  ARG A 217    12.848  27.823   3.451  1.00 30.82  A N
ATOM 1460  CZ  ARG A 217    12.770  27.401   4.711  1.00 30.65  A C
ATOM 1461  NH1 ARG A 217    12.167  26.252   4.987  1.00 31.00  A N
ATOM 1462  NH2 ARG A 217    13.283  28.128   5.696  1.00 30.57  A N
ATOM 1463  C   ARG A 217     8.662  30.393   1.449  1.00 29.98  A C
ATOM 1464  O   ARG A 217     9.102  31.044   0.498  1.00 30.07  A O
ATOM 1465  N   TYR A 218     8.002  30.951   2.460  1.00 29.02  A N
ATOM 1466  CA  TYR A 218     7.764  32.391   2.507  1.00 27.95  A C
ATOM 1467  CB  TYR A 218     6.624  32.788   1.559  1.00 27.52  A C
ATOM 1468  CG  TYR A 218     5.277  32.204   1.934  1.00 27.07  A C
ATOM 1469  CD1 TYR A 218     4.385  32.904   2.760  1.00 26.70  A C
ATOM 1470  CE1 TYR A 218     3.149  32.359   3.112  1.00 26.51  A C
ATOM 1471  CD2 TYR A 218     4.895  30.941   1.472  1.00 27.02  A C
ATOM 1472  CE2 TYR A 218     3.664  30.389   1.820  1.00 26.80  A C
ATOM 1473  CZ  TYR A 218     2.797  31.099   2.637  1.00 26.82  A C
ATOM 1474  OH  TYR A 218     1.580  30.538   2.969  1.00 26.94  A O
ATOM 1475  C   TYR A 218     7.405  32.801   3.918  1.00 27.50  A C
ATOM 1476  O   TYR A 218     6.998  31.972   4.731  1.00 27.62  A O
ATOM 1477  N   HIS A 219     7.576  34.080   4.219  1.00 26.81  A N
ATOM 1478  CA  HIS A 219     7.208  34.568   5.528  1.00 26.29  A C
ATOM 1479  CB  HIS A 219     8.365  35.339   6.170  1.00 26.16  A C
ATOM 1480  CG  HIS A 219     9.426  34.436   6.727  1.00 26.51  A C
ATOM 1481  CD2 HIS A 219     9.603  33.929   7.971  1.00 26.77  A C
ATOM 1482  ND1 HIS A 219    10.405  33.865   5.944  1.00 27.13  A N
ATOM 1483  CE1 HIS A 219    11.141  33.047   6.676  1.00 26.96  A C
ATOM 1484  NE2 HIS A 219    10.675  33.067   7.911  1.00 26.74  A N
ATOM 1485  C   HIS A 219     5.928  35.385   5.356  1.00 25.76  A C
ATOM 1486  O   HIS A 219     5.684  35.961   4.302  1.00 25.37  A O
ATOM 1487  N   GLY A 220     5.103  35.375   6.390  1.00 25.33  A N
ATOM 1488  CA  GLY A 220     3.813  36.027   6.339  1.00 25.21  A C
ATOM 1489  C   GLY A 220     3.672  37.437   5.819  1.00 25.15  A C
ATOM 1490  O   GLY A 220     3.052  37.675   4.782  1.00 24.85  A O
ATOM 1491  N   ARG A 221     4.250  38.375   6.556  1.00 25.21  A N
ATOM 1492  CA  ARG A 221     4.163  39.775   6.226  1.00 25.18  A C
ATOM 1493  CB  ARG A 221     4.799  40.564   7.368  1.00 26.41  A C
ATOM 1494  CG  ARG A 221     4.350  40.007   8.736  1.00 28.87  A C
ATOM 1495  CD  ARG A 221     4.942  40.735   9.946  1.00 30.80  A C
ATOM 1496  NE  ARG A 221     4.481  40.198  11.242  1.00 32.45  A N
ATOM 1497  CZ  ARG A 221     5.076  39.206  11.920  1.00 33.77  A C
ATOM 1498  NH1 ARG A 221     6.169  38.612  11.433  1.00 34.15  A N
ATOM 1499  NH2 ARG A 221     4.618  38.833  13.124  1.00 34.26  A N
ATOM 1500  C   ARG A 221     4.759  40.144   4.869  1.00 24.52  A C
ATOM 1501  O   ARG A 221     4.129  40.872   4.088  1.00 24.35  A O
ATOM 1502  N   SER A 222     5.947  39.636   4.562  1.00 23.44  A N
ATOM 1503  CA  SER A 222     6.562  39.983   3.288  1.00 22.87  A C
ATOM 1504  CB  SER A 222     8.043  39.588   3.295  1.00 22.75  A C
ATOM 1505  OG  SER A 222     8.197  38.182   3.332  1.00 23.38  A O
ATOM 1506  C   SER A 222     5.817  39.347   2.090  1.00 22.47  A C
ATOM 1507  O   SER A 222     5.828  39.885   0.989  1.00 22.59  A O
ATOM 1508  N   ALA A 223     5.181  38.202   2.298  1.00 21.84  A N
ATOM 1509  CA  ALA A 223     4.424  37.581   1.217  1.00 21.55  A C
ATOM 1510  CB  ALA A 223     4.029  36.142   1.585  1.00 21.28  A C
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FIGURE 2A-28

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ATOM 1511  C   ALA A 223     3.164  38.430   1.011  1.00 21.38  A C
ATOM 1512  O   ALA A 223     2.698  38.601  -0.121  1.00 20.82  A O
ATOM 1513  N   ALA A 224     2.619  38.961   2.111  1.00 20.87  A N
ATOM 1514  CA  ALA A 224     1.419  39.788   2.022  1.00 20.64  A C
ATOM 1515  CB  ALA A 224     0.908  40.112   3.397  1.00 20.36  A C
ATOM 1516  C   ALA A 224     1.704  41.077   1.254  1.00 20.54  A C
ATOM 1517  O   ALA A 224     0.891  41.516   0.433  1.00 20.69  A O
ATOM 1518  N   VAL A 225     2.866  41.669   1.523  1.00 20.31  A N
ATOM 1519  CA  VAL A 225     3.280  42.908   0.881  1.00 19.98  A C
ATOM 1520  CB  VAL A 225     4.631  43.412   1.496  1.00 19.99  A C
ATOM 1521  CG1 VAL A 225     5.232  44.549   0.661  1.00 19.15  A C
ATOM 1522  CG2 VAL A 225     4.380  43.893   2.928  1.00 19.94  A C
ATOM 1523  C   VAL A 225     3.397  42.697  -0.629  1.00 20.24  A C
ATOM 1524  O   VAL A 225     2.993  43.564  -1.411  1.00 20.22  A O
ATOM 1525  N   TRP A 226     3.942  41.550  -1.045  1.00 20.02  A N
ATOM 1526  CA  TRP A 226     4.051  41.248  -2.471  1.00 19.92  A C
ATOM 1527  CB  TRP A 226     4.753  39.896  -2.691  1.00 20.44  A C
ATOM 1528  CG  TRP A 226     4.700  39.401  -4.124  1.00 20.89  A C
ATOM 1529  CD2 TRP A 226     5.729  39.536  -5.118  1.00 21.22  A C
ATOM 1530  CE2 TRP A 226     5.238  38.954  -6.314  1.00 21.15  A C
ATOM 1531  CE3 TRP A 226     7.018  40.093  -5.113  1.00 21.45  A C
ATOM 1532  CD1 TRP A 226     3.657  38.756  -4.740  1.00 21.03  A C
ATOM 1533  NE1 TRP A 226     3.975  38.484  -6.057  1.00 21.38  A N
ATOM 1534  CZ2 TRP A 226     5.989  38.913  -7.492  1.00 21.46  A C
ATOM 1535  CZ3 TRP A 226     7.767  40.052  -6.292  1.00 22.03  A C
ATOM 1536  CH2 TRP A 226     7.245  39.464  -7.465  1.00 21.80  A C
ATOM 1537  C   TRP A 226     2.654  41.195  -3.099  1.00 19.83  A C
ATOM 1538  O   TRP A 226     2.425  41.775  -4.150  1.00 19.96  A O
ATOM 1539  N   SER A 227     1.718  40.493  -2.468  1.00 19.51  A N
ATOM 1540  CA  SER A 227     0.377  40.409  -3.033  1.00 19.57  A C
ATOM 1541  CB  SER A 227    -0.491  39.459  -2.215  1.00 19.33  A C
ATOM 1542  OG  SER A 227    -0.858  40.041  -0.983  1.00 20.33  A O
ATOM 1543  C   SER A 227    -0.256  41.801  -3.088  1.00 19.65  A C
ATOM 1544  O   SER A 227    -1.063  42.086  -3.970  1.00 19.43  A O
ATOM 1545  N   LEU A 228     0.106  42.666  -2.140  1.00 19.63  A N
ATOM 1546  CA  LEU A 228    -0.416  44.026  -2.134  1.00 19.91  A C
ATOM 1547  CB  LEU A 228    -0.080  44.729  -0.805  1.00 19.98  A C
ATOM 1548  CG  LEU A 228    -0.911  44.251   0.400  1.00 20.23  A C
ATOM 1549  CD1 LEU A 228    -0.355  44.818   1.703  1.00 20.22  A C
ATOM 1550  CD2 LEU A 228    -2.377  44.680   0.202  1.00 20.05  A C
ATOM 1551  C   LEU A 228     0.174  44.790  -3.331  1.00 19.92  A C
ATOM 1552  O   LEU A 228    -0.466  45.678  -3.883  1.00 19.91  A O
ATOM 1553  N   GLY A 229     1.384  44.428  -3.747  1.00 19.78  A N
ATOM 1554  CA  GLY A 229     1.981  45.086  -4.897  1.00 19.76  A C
ATOM 1555  C   GLY A 229     1.259  44.691  -6.178  1.00 19.93  A C
ATOM 1556  O   GLY A 229     1.076  45.514  -7.086  1.00 19.49  A O
ATOM 1557  N   ILE A 230     0.840  43.428  -6.248  1.00 20.24  A N
ATOM 1558  CA  ILE A 230     0.116  42.911  -7.409  1.00 20.77  A C
ATOM 1559  CB  ILE A 230    -0.160  41.391  -7.276  1.00 21.07  A C
ATOM 1560  CG2 ILE A 230    -0.964  40.900  -8.481  1.00 20.87  A C
ATOM 1561  CG1 ILE A 230     1.155  40.616  -7.157  1.00 21.31  A C
ATOM 1562  CD1 ILE A 230     2.017  40.655  -8.412  1.00 21.99  A C
ATOM 1563  C   ILE A 230    -1.231  43.634  -7.451  1.00 20.96  A C
ATOM 1564  O   ILE A 230    -1.671  44.119  -8.496  1.00 20.41  A O
ATOM 1565  N   LEU A 231    -1.870  43.709  -6.288  1.00 21.10  A N
ATOM 1566  CA  LEU A 231    -3.160  44.371  -6.167  1.00 21.66  A C
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FIGURE 2A-29

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ATOM 1567  CB  LEU A 231    -3.641  44.313  -4.717  1.00 21.59  A C
ATOM 1568  CG  LEU A 231    -4.923  45.102  -4.418  1.00 21.98  A C
ATOM 1569  CD1 LEU A 231    -6.115  44.467  -5.156  1.00 21.81  A C
ATOM 1570  CD2 LEU A 231    -5.162  45.126  -2.900  1.00 21.45  A C
ATOM 1571  C   LEU A 231    -3.115  45.834  -6.622  1.00 21.80  A C
ATOM 1572  O   LEU A 231    -3.990  46.292  -7.352  1.00 22.19  A O
ATOM 1573  N   LEU A 232    -2.096  46.563  -6.188  1.00 21.72  A N
ATOM 1574  CA  LEU A 232    -1.969  47.969  -6.531  1.00 21.57  A C
ATOM 1575  CB  LEU A 232    -0.797  48.594  -5.764  1.00 21.93  A C
ATOM 1576  CG  LEU A 232    -0.896  50.072  -5.358  1.00 23.20  A C
ATOM 1577  CD1 LEU A 232     0.518  50.660  -5.169  1.00 22.55  A C
ATOM 1578  CD2 LEU A 232    -1.698  50.861  -6.385  1.00 22.62  A C
ATOM 1579  C   LEU A 232    -1.754  48.138  -8.037  1.00 21.43  A C
ATOM 1580  O   LEU A 232    -2.353  49.020  -8.673  1.00 21.28  A O
ATOM 1581  N   TYR A 233    -0.893  47.306  -8.610  1.00 20.83  A N
ATOM 1582  CA  TYR A 233    -0.646  47.376 -10.041  1.00 20.65  A C
ATOM 1583  CB  TYR A 233     0.419  46.338 -10.442  1.00 20.34  A C
ATOM 1584  CG  TYR A 233     0.724  46.267 -11.937  1.00 20.14  A C
ATOM 1585  CD1 TYR A 233    -0.163  45.657 -12.813  1.00 19.91  A C
ATOM 1586  CE1 TYR A 233     0.066  45.643 -14.197  1.00 20.15  A C
ATOM 1587  CD2 TYR A 233     1.874  46.864 -12.467  1.00 19.65  A C
ATOM 1588  CE2 TYR A 233     2.120  46.864 -13.851  1.00 20.41  A C
ATOM 1589  CZ  TYR A 233     1.199  46.251 -14.712  1.00 20.36  A C
ATOM 1590  OH  TYR A 233     1.389  46.271 -16.079  1.00 20.44  A O
ATOM 1591  C   TYR A 233    -1.982  47.102 -10.741  1.00 20.78  A C
ATOM 1592  O   TYR A 233    -2.356  47.794 -11.684  1.00 21.23  A O
ATOM 1593  N   ASP A 234    -2.694  46.090 -10.267  1.00 20.79  A N
ATOM 1594  CA  ASP A 234    -3.992  45.709 -10.822  1.00 21.48  A C
ATOM 1595  CB  ASP A 234    -4.617  44.623  -9.950  1.00 21.66  A C
ATOM 1596  CG  ASP A 234    -5.945  44.118 -10.491  1.00 22.42  A C
ATOM 1597  OD1 ASP A 234    -6.869  43.947  -9.678  1.00 22.96  A O
ATOM 1598  OD2 ASP A 234    -6.072  43.871 -11.709  1.00 22.23  A O
ATOM 1599  C   ASP A 234    -4.924  46.922 -10.849  1.00 21.94  A C
ATOM 1600  O   ASP A 234    -5.552  47.210 -11.869  1.00 22.08  A O
ATOM 1601  N   MET A 235    -4.994  47.629  -9.724  1.00 22.03  A N
ATOM 1602  CA  MET A 235    -5.841  48.795  -9.611  1.00 22.98  A C
ATOM 1603  CB  MET A 235    -5.795  49.385  -8.195  1.00 23.37  A C
ATOM 1604  CG  MET A 235    -6.540  48.647  -7.137  1.00 24.11  A C
ATOM 1605  SD  MET A 235    -6.343  49.513  -5.592  1.00 25.96  A S
ATOM 1606  CE  MET A 235    -7.036  48.337  -4.560  1.00 25.71  A C
ATOM 1607  C   MET A 235    -5.458  49.906 -10.579  1.00 23.19  A C
ATOM 1608  O   MET A 235    -6.322  50.483 -11.221  1.00 23.42  A O
ATOM 1609  N   VAL A 236    -4.174  50.205 -10.706  1.00 23.39  A N
ATOM 1610  CA  VAL A 236    -3.798  51.309 -11.575  1.00 23.80  A C
ATOM 1611  CB  VAL A 236    -2.532  52.041 -11.051  1.00 23.52  A C
ATOM 1612  CG1 VAL A 236    -2.825  52.640  -9.667  1.00 23.41  A C
ATOM 1613  CG2 VAL A 236    -1.353  51.085 -11.003  1.00 22.95  A C
ATOM 1614  C   VAL A 236    -3.612  50.991 -13.039  1.00 24.33  A C
ATOM 1615  O   VAL A 236    -3.553  51.916 -13.848  1.00 24.47  A O
ATOM 1616  N   CYS A 237    -3.526  49.711 -13.394  1.00 24.96  A N
ATOM 1617  CA  CYS A 237    -3.351  49.351 -14.797  1.00 25.93  A C
ATOM 1618  CB  CYS A 237    -2.098  48.499 -14.978  1.00 26.03  A C
ATOM 1619  SG  CYS A 237    -0.572  49.426 -14.693  1.00 27.34  A S
ATOM 1620  C   CYS A 237    -4.557  48.615 -15.360  1.00 26.45  A C
ATOM 1621  O   CYS A 237    -4.694  48.478 -16.574  1.00 26.36  A O
ATOM 1622  N   GLY A 238    -5.431  48.142 -14.477  1.00 26.89  A N
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FIGURE 2A-30

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ATOM 1623  CA  GLY A 238    -6.610  47.439 -14.941  1.00 27.79  A C
ATOM 1624  C   GLY A 238    -6.442  45.939 -15.046  1.00 28.38  A C
ATOM 1625  O   GLY A 238    -7.397  45.237 -15.343  1.00 28.58  A O
ATOM 1626  N   ASP A 239    -5.235  45.441 -14.809  1.00 29.03  A N
ATOM 1627  CA  ASP A 239    -4.984  44.005 -14.859  1.00 29.80  A C
ATOM 1628  CB  ASP A 239    -4.803  43.556 -16.311  1.00 30.68  A C
ATOM 1629  CG  ASP A 239    -5.241  42.115 -16.538  1.00 32.06  A C
ATOM 1630  OD1 ASP A 239    -5.477  41.377 -15.545  1.00 31.91  A O
ATOM 1631  OD2 ASP A 239    -5.342  41.714 -17.732  1.00 33.33  A O
ATOM 1632  C   ASP A 239    -3.722  43.672 -14.046  1.00 29.86  A C
ATOM 1633  O   ASP A 239    -2.946  44.567 -13.725  1.00 29.61  A O
ATOM 1634  N   ILE A 240    -3.526  42.397 -13.710  1.00 30.02  A N
ATOM 1635  CA  ILE A 240    -2.357  41.996 -12.940  1.00 30.43  A C
ATOM 1636  CB  ILE A 240    -2.521  40.590 -12.330  1.00 30.48  A C
ATOM 1637  CG2 ILE A 240    -3.612  40.608 -11.306  1.00 30.30  A C
ATOM 1638  CG1 ILE A 240    -2.824  39.557 -13.417  1.00 30.75  A C
ATOM 1639  CD1 ILE A 240    -3.172  38.174 -12.853  1.00 30.65  A C
ATOM 1640  C   ILE A 240    -1.107  42.051 -13.816  1.00 30.71  A C
ATOM 1641  O   ILE A 240    -1.185  41.935 -15.041  1.00 30.63  A O
ATOM 1642  N   PRO A 241     0.065  42.248 -13.195  1.00 30.90  A N
ATOM 1643  CD  PRO A 241     0.263  42.401 -11.740  1.00 30.69  A C
ATOM 1644  CA  PRO A 241     1.345  42.340 -13.903  1.00 31.22  A C
ATOM 1645  CB  PRO A 241     2.256  42.988 -12.864  1.00 30.69  A C
ATOM 1646  CG  PRO A 241     1.780  42.365 -11.599  1.00 30.54  A C
ATOM 1647  C   PRO A 241     1.941  41.048 -14.445  1.00 31.70  A C
ATOM 1648  O   PRO A 241     2.576  41.052 -15.499  1.00 31.53  A O
ATOM 1649  N   PHE A 242     1.734  39.948 -13.730  1.00 32.38  A N
ATOM 1650  CA  PHE A 242     2.315  38.673 -14.130  1.00 33.18  A C
ATOM 1651  CB  PHE A 242     3.289  38.173 -13.056  1.00 32.46  A C
ATOM 1652  CG  PHE A 242     4.217  39.224 -12.527  1.00 32.00  A C
ATOM 1653  CD1 PHE A 242     5.030  39.957 -13.387  1.00 32.01  A C
ATOM 1654  CD2 PHE A 242     4.326  39.442 -11.156  1.00 31.90  A C
ATOM 1655  CE1 PHE A 242     5.948  40.892 -12.888  1.00 31.67  A C
ATOM 1656  CE2 PHE A 242     5.239  40.377 -10.645  1.00 31.75  A C
ATOM 1657  CZ  PHE A 242     6.051  41.099 -11.518  1.00 31.72  A C
ATOM 1658  C   PHE A 242     1.283  37.588 -14.358  1.00 34.17  A C
ATOM 1659  O   PHE A 242     0.263  37.536 -13.677  1.00 34.02  A O
ATOM 1660  N   GLU A 243     1.578  36.701 -15.306  1.00 35.68  A N
ATOM 1661  CA  GLU A 243     0.690  35.592 -15.621  1.00 37.17  A C
ATOM 1662  CB  GLU A 243     0.191  35.718 -17.058  1.00 38.37  A C
ATOM 1663  CG  GLU A 243    -0.773  34.623 -17.429  1.00 40.46  A C
ATOM 1664  CD  GLU A 243    -1.981  34.597 -16.509  1.00 41.75  A C
ATOM 1665  OE1 GLU A 243    -2.484  33.479 -16.244  1.00 42.90  A O
ATOM 1666  OE2 GLU A 243    -2.434  35.683 -16.058  1.00 42.14  A O
ATOM 1667  C   GLU A 243     1.381  34.229 -15.420  1.00 37.44  A C
ATOM 1668  O   GLU A 243     0.783  33.290 -14.885  1.00 37.69  A O
ATOM 1669  N   HIS A 244     2.640  34.125 -15.832  1.00 37.59  A N
ATOM 1670  CA  HIS A 244     3.371  32.871 -15.687  1.00 37.73  A C
ATOM 1671  CB  HIS A 244     4.007  32.488 -17.022  1.00 38.67  A C
ATOM 1672  CG  HIS A 244     3.034  32.488 -18.157  1.00 39.71  A C
ATOM 1673  CD2 HIS A 244     2.018  31.643 -18.455  1.00 40.05  A C
ATOM 1674  ND1 HIS A 244     2.972  33.508 -19.084  1.00 40.21  A N
ATOM 1675  CE1 HIS A 244     1.955  33.293 -19.902  1.00 40.42  A C
ATOM 1676  NE2 HIS A 244     1.360  32.169 -19.541  1.00 40.43  A N
ATOM 1677  C   HIS A 244     4.439  32.912 -14.607  1.00 37.28  A C
ATOM 1678  O   HIS A 244     4.936  33.980 -14.240  1.00 37.01  A O
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FIGURE 2A-31

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ATOM 1679  N   ASP A 245     4.781  31.729 -14.106  1.00 36.91  A N
ATOM 1680  CA  ASP A 245     5.797  31.580 -13.075  1.00 36.71  A C
ATOM 1681  CB  ASP A 245     6.093  30.099 -12.831  1.00 36.91  A C
ATOM 1682  CG  ASP A 245     4.953  29.376 -12.153  1.00 37.13  A C
ATOM 1683  OD1 ASP A 245     3.974  30.034 -11.757  1.00 37.37  A O
ATOM 1684  OD2 ASP A 245     5.042  28.139 -12.004  1.00 37.45  A O
ATOM 1685  C   ASP A 245     7.099  32.284 -13.449  1.00 36.37  A C
ATOM 1686  O   ASP A 245     7.727  32.910 -12.603  1.00 36.07  A O
ATOM 1687  N   GLU A 246     7.505  32.181 -14.711  1.00 36.32  A N
ATOM 1688  CA  GLU A 246     8.752  32.809 -15.150  1.00 36.57  A C
ATOM 1689  CB  GLU A 246     9.075  32.449 -16.603  1.00 37.61  A C
ATOM 1690  CG  GLU A 246     8.785  31.014 -16.942  1.00 39.64  A C
ATOM 1691  CD  GLU A 246     7.297  30.766 -17.042  1.00 40.62  A C
ATOM 1692  OE1 GLU A 246     6.653  31.497 -17.822  1.00 41.69  A O
ATOM 1693  OE2 GLU A 246     6.772  29.859 -16.356  1.00 41.20  A O
ATOM 1694  C   GLU A 246     8.723  34.325 -15.009  1.00 35.88  A C
ATOM 1695  O   GLU A 246     9.747  34.941 -14.737  1.00 35.51  A O
ATOM 1696  N   GLU A 247     7.557  34.929 -15.203  1.00 35.34  A N
ATOM 1697  CA  GLU A 247     7.459  36.381 -15.063  1.00 35.07  A C
ATOM 1698  CB  GLU A 247     6.144  36.896 -15.628  1.00 35.57  A C
ATOM 1699  CG  GLU A 247     5.958  36.634 -17.090  1.00 36.98  A C
ATOM 1700  CD  GLU A 247     4.575  37.029 -17.539  1.00 37.87  A C
ATOM 1701  OE1 GLU A 247     3.590  36.422 -17.061  1.00 38.25  A O
ATOM 1702  OE2 GLU A 247     4.469  37.959 -18.356  1.00 38.77  A O
ATOM 1703  C   GLU A 247     7.545  36.766 -13.593  1.00 34.05  A C
ATOM 1704  O   GLU A 247     8.173  37.764 -13.244  1.00 33.72  A O
ATOM 1705  N   ILE A 248     6.913  35.970 -12.739  1.00 33.26  A N
ATOM 1706  CA  ILE A 248     6.937  36.242 -11.309  1.00 32.78  A C
ATOM 1707  CB  ILE A 248     6.109  35.200 -10.501  1.00 32.24  A C
ATOM 1708  CG2 ILE A 248     6.351  35.386  -9.001  1.00 31.56  A C
ATOM 1709  CG1 ILE A 248     4.625  35.348 -10.834  1.00 31.76  A C
ATOM 1710  CD1 ILE A 248     3.726  34.293 -10.212  1.00 31.59  A C
ATOM 1711  C   ILE A 248     8.368  36.233 -10.798  1.00 32.81  A C
ATOM 1712  O   ILE A 248     8.795  37.176 -10.114  1.00 32.44  A O
ATOM 1713  N   ILE A 249     9.128  35.191 -11.135  1.00 33.07  A N
ATOM 1714  CA  ILE A 249    10.497  35.145 -10.642  1.00 33.44  A C
ATOM 1715  CB  ILE A 249    11.117  33.701 -10.688  1.00 33.72  A C
ATOM 1716  CG2 ILE A 249    10.148  32.695 -10.069  1.00 33.43  A C
ATOM 1717  CG1 ILE A 249    11.446  33.281 -12.111  1.00 33.87  A C
ATOM 1718  CD1 ILE A 249    12.115  31.923 -12.160  1.00 34.83  A C
ATOM 1719  C   ILE A 249    11.416  36.158 -11.324  1.00 33.55  A C
ATOM 1720  O   ILE A 249    12.393  36.577 -10.709  1.00 33.80  A O
ATOM 1721  N   ARG A 250    11.117  36.563 -12.565  1.00 33.46  A N
ATOM 1722  CA  ARG A 250    11.944  37.568 -13.241  1.00 33.83  A C
ATOM 1723  CB  ARG A 250    11.529  37.731 -14.712  1.00 33.99  A C
ATOM 1724  CG  ARG A 250    12.342  38.754 -15.452  1.00 34.86  A C
ATOM 1725  CD  ARG A 250    12.638  38.329 -16.849  1.00 35.54  A C
ATOM 1726  NE  ARG A 250    13.182  39.413 -17.657  1.00 36.63  A N
ATOM 1727  CZ  ARG A 250    12.489  40.321 -18.353  1.00 36.92  A C
ATOM 1728  NH1 ARG A 250    11.158  40.356 -18.396  1.00 36.47  A N
ATOM 1729  NH2 ARG A 250    13.175  41.216 -19.040  1.00 37.45  A N
ATOM 1730  C   ARG A 250    11.721  38.876 -12.480  1.00 33.88  A C
ATOM 1731  O   ARG A 250    12.645  39.673 -12.270  1.00 33.90  A O
ATOM 1732  N   GLY A 251    10.469  39.070 -12.079  1.00 33.73  A N
ATOM 1733  CA  GLY A 251    10.088  40.234 -11.310  1.00 33.72  A C
ATOM 1734  C   GLY A 251    10.156  41.591 -11.978  1.00 33.70  A C
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FIGURE 2A-32

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ATOM 1735  O   GLY A 251   10.078  42.604 -11.283  1.00 34.00  A O
ATOM 1736  N   GLN A 252   10.317  41.658 -13.296  1.00 33.52  A N
ATOM 1737  CA  GLN A 252   10.348  42.976 -13.932  1.00 33.25  A C
ATOM 1738  CB  GLN A 252   11.186  42.982 -15.207  1.00 33.90  A C
ATOM 1739  CG  GLN A 252   12.667  43.024 -14.915  1.00 35.25  A C
ATOM 1740  CD  GLN A 252   13.481  43.478 -16.101  1.00 36.18  A C
ATOM 1741  OE1 GLN A 252   13.279  44.580 -16.630  1.00 36.77  A O
ATOM 1742  NE2 GLN A 252   14.417  42.634 -16.531  1.00 36.67  A N
ATOM 1743  C   GLN A 252    8.940  43.439 -14.239  1.00 32.60  A C
ATOM 1744  O   GLN A 252    8.149  42.723 -14.847  1.00 32.43  A O
ATOM 1745  N   VAL A 253    8.636  44.648 -13.799  1.00 32.00  A N
ATOM 1746  CA  VAL A 253    7.317  45.216 -13.987  1.00 31.51  A C
ATOM 1747  CB  VAL A 253    6.893  46.011 -12.734  1.00 31.25  A C
ATOM 1748  CG1 VAL A 253    5.515  46.592 -12.921  1.00 30.52  A C
ATOM 1749  CG2 VAL A 253    6.939  45.102 -11.517  1.00 31.64  A C
ATOM 1750  C   VAL A 253    7.231  46.145 -15.183  1.00 31.26  A C
ATOM 1751  O   VAL A 253    7.956  47.127 -15.268  1.00 31.36  A O
ATOM 1752  N   PHE A 254    6.331  45.839 -16.098  1.00 31.20  A N
ATOM 1753  CA  PHE A 254    6.124  46.684 -17.259  1.00 31.40  A C
ATOM 1754  CB  PHE A 254    6.115  45.835 -18.537  1.00 31.58  A C
ATOM 1755  CG  PHE A 254    5.605  46.576 -19.736  1.00 32.53  A C
ATOM 1756  CD1 PHE A 254    4.237  46.610 -20.025  1.00 32.57  A C
ATOM 1757  CD2 PHE A 254    6.476  47.315 -20.538  1.00 32.61  A C
ATOM 1758  CE1 PHE A 254    3.753  47.378 -21.093  1.00 32.96  A C
ATOM 1759  CE2 PHE A 254    5.993  48.085 -21.608  1.00 32.49  A C
ATOM 1760  CZ  PHE A 254    4.639  48.116 -21.882  1.00 32.33  A C
ATOM 1761  C   PHE A 254    4.779  47.398 -17.082  1.00 31.29  A C
ATOM 1762  O   PHE A 254    3.785  46.756 -16.755  1.00 31.45  A O
ATOM 1763  N   PHE A 255    4.737  48.714 -17.279  1.00 31.00  A N
ATOM 1764  CA  PHE A 255    3.476  49.443 -17.132  1.00 31.15  A C
ATOM 1765  CB  PHE A 255    3.705  50.779 -16.421  1.00 30.06  A C
ATOM 1766  CG  PHE A 255    3.921  50.632 -14.949  1.00 29.23  A C
ATOM 1767  CD1 PHE A 255    5.179  50.319 -14.446  1.00 28.55  A C
ATOM 1768  CD2 PHE A 255    2.837  50.708 -14.066  1.00 28.82  A C
ATOM 1769  CE1 PHE A 255    5.365  50.074 -13.095  1.00 28.37  A C
ATOM 1770  CE2 PHE A 255    3.010  50.466 -12.712  1.00 28.31  A C
ATOM 1771  CZ  PHE A 255    4.273  50.146 -12.221  1.00 28.44  A C
ATOM 1772  C   PHE A 255    2.737  49.666 -18.446  1.00 31.69  A C
ATOM 1773  O   PHE A 255    3.240  50.330 -19.347  1.00 31.81  A O
ATOM 1774  N   ARG A 256    1.536  49.103 -18.542  1.00 32.57  A N
ATOM 1775  CA  ARG A 256    0.721  49.208 -19.753  1.00 33.38  A C
ATOM 1776  CB  ARG A 256   -0.159  47.950 -19.902  1.00 34.40  A C
ATOM 1777  CG  ARG A 256   -0.975  47.587 -18.653  1.00 35.95  A C
ATOM 1778  CD  ARG A 256   -1.887  46.373 -18.903  1.00 37.38  A C
ATOM 1779  NE  ARG A 256   -1.176  45.090 -18.951  1.00 38.60  A N
ATOM 1780  CZ  ARG A 256   -0.995  44.286 -17.901  1.00 38.94  A C
ATOM 1781  NH1 ARG A 256   -1.476  44.626 -16.715  1.00 39.57  A N
ATOM 1782  NH2 ARG A 256   -0.330  43.146 -18.029  1.00 38.97  A N
ATOM 1783  C   ARG A 256   -0.153  50.455 -19.780  1.00 33.11  A C
ATOM 1784  O   ARG A 256   -0.785  50.754 -20.786  1.00 33.46  A O
ATOM 1785  N   GLN A 257   -0.176  51.181 -18.669  1.00 32.72  A N
ATOM 1786  CA  GLN A 257   -0.973  52.395 -18.538  1.00 32.11  A C
ATOM 1787  CB  GLN A 257   -2.165  52.148 -17.600  1.00 33.44  A C
ATOM 1788  CG  GLN A 257   -3.142  51.069 -18.037  1.00 35.31  A C
ATOM 1789  CD  GLN A 257   -4.067  51.553 -19.132  1.00 36.64  A C
ATOM 1790  OE1 GLN A 257   -4.653  52.638 -19.028  1.00 37.18  A O
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FIGURE 2A-33

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ATOM 1791  NE2 GLN A 257    -4.209  50.751 -20.192  1.00 37.39  A N
ATOM 1792  C   GLN A 257    -0.115  53.504 -17.925  1.00 31.03  A C
ATOM 1793  O   GLN A 257     0.894  53.235 -17.276  1.00 30.46  A O
ATOM 1794  N   ARG A 258    -0.533  54.747 -18.120  1.00 29.82  A N
ATOM 1795  CA  ARG A 258     0.180  55.877 -17.558  1.00 29.07  A C
ATOM 1796  CB  ARG A 258    -0.381  57.182 -18.115  1.00 29.25  A C
ATOM 1797  CG  ARG A 258     0.544  58.348 -17.936  1.00 29.72  A C
ATOM 1798  CD  ARG A 258     0.541  58.874 -16.530  1.00 30.84  A C
ATOM 1799  NE  ARG A 258     1.702  59.730 -16.323  1.00 31.85  A N
ATOM 1800  CZ  ARG A 258     1.953  60.421 -15.214  1.00 32.93  A C
ATOM 1801  NH1 ARG A 258     1.109  60.374 -14.170  1.00 33.10  A N
ATOM 1802  NH2 ARG A 258     3.062  61.158 -15.145  1.00 32.87  A N
ATOM 1803  C   ARG A 258     0.021  55.858 -16.036  1.00 28.35  A C
ATOM 1804  O   ARG A 258    -1.093  55.928 -15.532  1.00 27.92  A O
ATOM 1805  N   VAL A 259     1.134  55.759 -15.319  1.00 27.52  A N
ATOM 1806  CA  VAL A 259     1.122  55.725 -13.865  1.00 27.05  A C
ATOM 1807  CB  VAL A 259     1.352  54.272 -13.343  1.00 27.08  A C
ATOM 1808  CG1 VAL A 259     1.436  54.251 -11.799  1.00 26.35  A C
ATOM 1809  CG2 VAL A 259     0.232  53.373 -13.817  1.00 26.53  A C
ATOM 1810  C   VAL A 259     2.242  56.636 -13.354  1.00 27.10  A C
ATOM 1811  O   VAL A 259     3.365  56.591 -13.863  1.00 26.84  A O
ATOM 1812  N   SER A 260     1.942  57.457 -12.354  1.00 26.98  A N
ATOM 1813  CA  SER A 260     2.940  58.377 -11.809  1.00 27.48  A C
ATOM 1814  CB  SER A 260     2.368  59.170 -10.628  1.00 26.89  A C
ATOM 1815  OG  SER A 260     2.116  58.330  -9.511  1.00 26.28  A O
ATOM 1816  C   SER A 260     4.205  57.666 -11.360  1.00 27.95  A C
ATOM 1817  O   SER A 260     4.176  56.489 -11.003  1.00 28.17  A O
ATOM 1818  N   PSR A 261     5.312  58.396 -11.375  1.00 28.70  A N
ATOM 1819  CA  PSR A 261     6.604  57.862 -10.971  1.00 29.59  A C
ATOM 1820  CB  PSR A 261     7.688  58.934 -11.161  1.00 31.24  A C
ATOM 1821  OG  PSR A 261     7.616  59.491 -12.511  1.00 34.22  A O
ATOM 1822  C   PSR A 261     6.567  57.388  -9.511  1.00 29.22  A C
ATOM 1823  O   PSR A 261     7.204  56.395  -9.153  1.00 29.05  A O
ATOM 1824  P   PSR A 261     6.823  61.050 -12.979  1.00 37.32  A P
ATOM 1825  O1  PSR A 261     7.451  62.297 -12.352  1.00 36.03  A O
ATOM 1826  O2  PSR A 261     7.088  61.056 -14.601  1.00 35.85  A O
ATOM 1827  O3  PSR A 261     5.247  61.006 -12.597  1.00 35.30  A O
ATOM 1828  N   GLU A 262     5.819  58.091  -8.668  1.00 28.88  A N
ATOM 1829  CA  GLU A 262     5.723  57.707  -7.263  1.00 28.67  A C
ATOM 1830  CB  GLU A 262     5.120  58.845  -6.428  1.00 29.89  A C
ATOM 1831  CG  GLU A 262     6.143  59.931  -6.101  1.00 32.10  A C
ATOM 1832  CD  GLU A 262     5.552  61.113  -5.359  1.00 33.87  A C
ATOM 1833  OE1 GLU A 262     6.334  62.036  -5.022  1.00 35.19  A O
ATOM 1834  OE2 GLU A 262     4.319  61.134  -5.115  1.00 34.79  A O
ATOM 1835  C   GLU A 262     4.931  56.420  -7.059  1.00 27.43  A C
ATOM 1836  O   GLU A 262     5.278  55.627  -6.195  1.00 27.16  A O
ATOM 1837  N   CYS A 263     3.877  56.214  -7.848  1.00 26.30  A N
ATOM 1838  CA  CYS A 263     3.082  54.997  -7.738  1.00 25.26  A C
ATOM 1839  CB  CYS A 263     1.778  55.112  -8.535  1.00 24.74  A C
ATOM 1840  SG  CYS A 263     0.611  53.714  -8.325  1.00 24.55  A S
ATOM 1841  C   CYS A 263     3.936  53.846  -8.266  1.00 24.99  A C
ATOM 1842  O   CYS A 263     4.035  52.804  -7.628  1.00 24.79  A O
ATOM 1843  N   GLN A 264     4.557  54.039  -9.426  1.00 24.65  A N
ATOM 1844  CA  GLN A 264     5.425  53.010  -9.991  1.00 24.72  A C
ATOM 1845  CB  GLN A 264     6.120  53.511 -11.265  1.00 24.67  A C
ATOM 1846  CG  GLN A 264     5.272  53.429 -12.528  1.00 24.85  A C
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FIGURE 2A-34

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ATOM 1847  CD  GLN A 264     6.096  53.666 -13.790  1.00 25.54  A C
ATOM 1848  OE1 GLN A 264     7.286  53.342 -13.833  1.00 25.78  A O
ATOM 1849  NE2 GLN A 264     5.462  54.207 -14.827  1.00 25.21  A N
ATOM 1850  C   GLN A 264     6.492  52.624  -8.968  1.00 24.61  A C
ATOM 1851  O   GLN A 264     6.845  51.449  -8.821  1.00 24.48  A O
ATOM 1852  N   HIS A 265     7.014  53.618  -8.261  1.00 24.42  A N
ATOM 1853  CA  HIS A 265     8.029  53.330  -7.269  1.00 24.66  A C
ATOM 1854  CB  HIS A 265     8.601  54.623  -6.685  1.00 25.32  A C
ATOM 1855  CG  HIS A 265     9.568  54.390  -5.567  1.00 26.67  A C
ATOM 1856  CD2 HIS A 265    10.894  54.102  -5.579  1.00 26.96  A C
ATOM 1857  ND1 HIS A 265     9.184  54.383  -4.243  1.00 27.00  A N
ATOM 1858  CE1 HIS A 265    10.233  54.102  -3.486  1.00 27.50  A C
ATOM 1859  NE2 HIS A 265    11.281  53.926  -4.273  1.00 27.52  A N
ATOM 1860  C   HIS A 265     7.474  52.438  -6.150  1.00 23.97  A C
ATOM 1861  O   HIS A 265     8.070  51.426  -5.818  1.00 23.59  A O
ATOM 1862  N   LEU A 266     6.330  52.805  -5.579  1.00 23.37  A N
ATOM 1863  CA  LEU A 266     5.741  51.995  -4.511  1.00 22.89  A C
ATOM 1864  CB  LEU A 266     4.438  52.641  -3.998  1.00 22.42  A C
ATOM 1865  CG  LEU A 266     3.705  51.916  -2.856  1.00 22.40  A C
ATOM 1866  CD1 LEU A 266     4.667  51.626  -1.695  1.00 21.72  A C
ATOM 1867  CD2 LEU A 266     2.539  52.777  -2.365  1.00 21.68  A C
ATOM 1868  C   LEU A 266     5.474  50.563  -5.004  1.00 22.67  A C
ATOM 1869  O   LEU A 266     5.739  49.594  -4.291  1.00 22.60  A O
ATOM 1870  N   ILE A 267     4.982  50.424  -6.229  1.00 22.27  A N
ATOM 1871  CA  ILE A 267     4.702  49.101  -6.761  1.00 22.30  A C
ATOM 1872  CB  ILE A 267     4.013  49.196  -8.137  1.00 21.95  A C
ATOM 1873  CG2 ILE A 267     4.023  47.840  -8.824  1.00 21.59  A C
ATOM 1874  CG1 ILE A 267     2.575  49.693  -7.961  1.00 21.55  A C
ATOM 1875  CD1 ILE A 267     1.861  50.038  -9.277  1.00 21.25  A C
ATOM 1876  C   ILE A 267     5.957  48.238  -6.886  1.00 22.81  A C
ATOM 1877  O   ILE A 267     5.962  47.066  -6.489  1.00 23.11  A O
ATOM 1878  N   ARG A 268     7.024  48.803  -7.430  1.00 23.08  A N
ATOM 1879  CA  ARG A 268     8.249  48.043  -7.592  1.00 23.64  A C
ATOM 1880  CB  ARG A 268     9.238  48.810  -8.489  1.00 24.18  A C
ATOM 1881  CG  ARG A 268     8.779  48.872  -9.935  1.00 24.60  A C
ATOM 1882  CD  ARG A 268     9.836  49.437 -10.847  1.00 25.54  A C
ATOM 1883  NE  ARG A 268     9.482  49.192 -12.247  1.00 26.34  A N
ATOM 1884  CZ  ARG A 268     9.052  50.128 -13.092  1.00 26.56  A C
ATOM 1885  NH1 ARG A 268     8.926  51.392 -12.691  1.00 26.63  A N
ATOM 1886  NH2 ARG A 268     8.727  49.793 -14.330  1.00 26.36  A N
ATOM 1887  C   ARG A 268     8.890  47.707  -6.257  1.00 23.61  A C
ATOM 1888  O   ARG A 268     9.600  46.710  -6.136  1.00 23.79  A O
ATOM 1889  N   TRP A 269     8.634  48.531  -5.248  1.00 23.51  A N
ATOM 1890  CA  TRP A 269     9.194  48.283  -3.927  1.00 23.53  A C
ATOM 1891  CB  TRP A 269     9.065  49.557  -3.065  1.00 23.84  A C
ATOM 1892  CG  TRP A 269     9.810  49.534  -1.747  1.00 24.35  A C
ATOM 1893  CD2 TRP A 269     9.707  50.496  -0.684  1.00 24.46  A C
ATOM 1894  CE2 TRP A 269    10.588  50.083   0.346  1.00 24.57  A C
ATOM 1895  CE3 TRP A 269     8.958  51.665  -0.502  1.00 24.77  A C
ATOM 1896  CD1 TRP A 269    10.729  48.601  -1.328  1.00 24.62  A C
ATOM 1897  NE1 TRP A 269    11.197  48.927  -0.071  1.00 24.37  A N
ATOM 1898  CZ2 TRP A 269    10.738  50.798   1.540  1.00 24.59  A C
ATOM 1899  CZ3 TRP A 269     9.109  52.381   0.694  1.00 25.02  A C
ATOM 1900  CH2 TRP A 269     9.994  51.940   1.697  1.00 24.80  A C
ATOM 1901  C   TRP A 269     8.449  47.074  -3.322  1.00 23.32  A C
ATOM 1902  O   TRP A 269     9.077  46.122  -2.844  1.00 23.39  A O
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FIGURE 2A-35

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ATOM 1903  N   CYS A 270     7.118  47.095  -3.367  1.00 22.88  A N
ATOM 1904  CA  CYS A 270     6.328  45.977  -2.847  1.00 22.48  A C
ATOM 1905  CB  CYS A 270     4.821  46.242  -3.016  1.00 22.41  A C
ATOM 1906  SG  CYS A 270     4.173  47.522  -1.929  1.00 23.18  A S
ATOM 1907  C   CYS A 270     6.683  44.683  -3.573  1.00 22.30  A C
ATOM 1908  O   CYS A 270     6.623  43.602  -2.987  1.00 22.05  A O
ATOM 1909  N   LEU A 271     7.066  44.792  -4.846  1.00 22.32  A N
ATOM 1910  CA  LEU A 271     7.416  43.608  -5.634  1.00 22.79  A C
ATOM 1911  CB  LEU A 271     6.852  43.740  -7.047  1.00 22.39  A C
ATOM 1912  CG  LEU A 271     5.335  43.941  -7.087  1.00 22.47  A C
ATOM 1913  CD1 LEU A 271     4.869  44.139  -8.535  1.00 21.83  A C
ATOM 1914  CD2 LEU A 271     4.649  42.714  -6.445  1.00 21.83  A C
ATOM 1915  C   LEU A 271     8.917  43.288  -5.710  1.00 23.18  A C
ATOM 1916  O   LEU A 271     9.371  42.643  -6.657  1.00 22.86  A O
ATOM 1917  N   ALA A 272     9.678  43.722  -4.710  1.00 23.63  A N
ATOM 1918  CA  ALA A 272    11.112  43.446  -4.695  1.00 24.38  A C
ATOM 1919  CB  ALA A 272    11.789  44.129  -3.490  1.00 24.22  A C
ATOM 1920  C   ALA A 272    11.271  41.937  -4.617  1.00 24.94  A C
ATOM 1921  O   ALA A 272    10.559  41.258  -3.865  1.00 24.37  A O
ATOM 1922  N   LEU A 273    12.193  41.427  -5.426  1.00 25.88  A N
ATOM 1923  CA  LEU A 273    12.487  40.008  -5.501  1.00 27.04  A C
ATOM 1924  CB  LEU A 273    13.612  39.786  -6.528  1.00 27.19  A C
ATOM 1925  CG  LEU A 273    13.279  39.024  -7.814  1.00 27.71  A C
ATOM 1926  CD1 LEU A 273    11.796  39.113  -8.123  1.00 27.34  A C
ATOM 1927  CD2 LEU A 273    14.133  39.568  -8.972  1.00 27.38  A C
ATOM 1928  C   LEU A 273    12.890  39.448  -4.135  1.00 27.55  A C
ATOM 1929  O   LEU A 273    12.421  38.387  -3.723  1.00 27.51  A O
ATOM 1930  N   ARG A 274    13.754  40.161  -3.427  1.00 28.36  A N
ATOM 1931  CA  ARG A 274    14.187  39.696  -2.116  1.00 29.64  A C
ATOM 1932  CB  ARG A 274    15.574  40.266  -1.777  1.00 31.22  A C
ATOM 1933  CG  ARG A 274    16.046  39.928  -0.356  1.00 34.10  A C
ATOM 1934  CD  ARG A 274    17.230  40.808   0.125  1.00 36.50  A C
ATOM 1935  NE  ARG A 274    18.539  40.398  -0.394  1.00 38.44  A N
ATOM 1936  CZ  ARG A 274    18.939  40.534  -1.657  1.00 39.72  A C
ATOM 1937  NH1 ARG A 274    18.139  41.077  -2.572  1.00 40.42  A N
ATOM 1938  NH2 ARG A 274    20.154  40.122  -2.012  1.00 40.52  A N
ATOM 1939  C   ARG A 274    13.159  40.130  -1.074  1.00 29.49  A C
ATOM 1940  O   ARG A 274    12.907  41.317  -0.908  1.00 29.62  A O
ATOM 1941  N   PRO A 275    12.547  39.168  -0.362  1.00 29.37  A N
ATOM 1942  CD  PRO A 275    12.807  37.720  -0.477  1.00 29.33  A C
ATOM 1943  CA  PRO A 275    11.537  39.447   0.669  1.00 29.42  A C
ATOM 1944  CB  PRO A 275    11.411  38.117   1.396  1.00 29.45  A C
ATOM 1945  CG  PRO A 275    11.654  37.117   0.293  1.00 29.48  A C
ATOM 1946  C   PRO A 275    11.897  40.584   1.630  1.00 29.65  A C
ATOM 1947  O   PRO A 275    11.075  41.468   1.893  1.00 29.60  A O
ATOM 1948  N   SER A 276    13.123  40.559   2.152  1.00 29.63  A N
ATOM 1949  CA  SER A 276    13.578  41.573   3.097  1.00 29.63  A C
ATOM 1950  CB  SER A 276    14.915  41.155   3.731  1.00 29.91  A C
ATOM 1951  OG  SER A 276    15.992  41.207   2.803  1.00 30.23  A O
ATOM 1952  C   SER A 276    13.716  42.959   2.472  1.00 29.65  A C
ATOM 1953  O   SER A 276    13.812  43.957   3.190  1.00 29.77  A O
ATOM 1954  N   ASP A 277    13.721  43.029   1.143  1.00 29.52  A N
ATOM 1955  CA  ASP A 277    13.837  44.315   0.454  1.00 29.25  A C
ATOM 1956  CB  ASP A 277    14.433  44.126  -0.939  1.00 30.03  A C
ATOM 1957  CG  ASP A 277    15.967  44.158  -0.953  1.00 30.62  A C
ATOM 1958  OD1 ASP A 277    16.551  43.717  -1.963  1.00 31.32  A O
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FIGURE 2A-36

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ATOM 1959  OD2 ASP A 277   16.587  44.624   0.018  1.00 30.75  A O
ATOM 1960  C   ASP A 277   12.479  45.009   0.308  1.00 28.97  A C
ATOM 1961  O   ASP A 277   12.419  46.157  -0.141  1.00 29.31  A O
ATOM 1962  N   ARG A 278   11.399  44.318   0.667  1.00 27.83  A N
ATOM 1963  CA  ARG A 278   10.059  44.888   0.558  1.00 27.29  A C
ATOM 1964  CB  ARG A 278    9.006  43.775   0.470  1.00 26.28  A C
ATOM 1965  CG  ARG A 278    9.108  42.973  -0.818  1.00 25.60  A C
ATOM 1966  CD  ARG A 278    8.281  41.683  -0.799  1.00 24.72  A C
ATOM 1967  NE  ARG A 278    8.865  40.736  -1.742  1.00 23.44  A N
ATOM 1968  CZ  ARG A 278    8.686  39.420  -1.724  1.00 23.02  A C
ATOM 1969  NH1 ARG A 278    7.913  38.844  -0.808  1.00 22.65  A N
ATOM 1970  NH2 ARG A 278    9.334  38.673  -2.601  1.00 22.37  A N
ATOM 1971  C   ARG A 278    9.753  45.787   1.737  1.00 27.20  A C
ATOM 1972  O   ARG A 278   10.350  45.656   2.801  1.00 27.45  A O
ATOM 1973  N   PRO A 279    8.818  46.725   1.563  1.00 27.16  A N
ATOM 1974  CD  PRO A 279    8.088  47.070   0.326  1.00 27.13  A C
ATOM 1975  CA  PRO A 279    8.462  47.632   2.652  1.00 27.11  A C
ATOM 1976  CB  PRO A 279    7.726  48.753   1.934  1.00 27.11  A C
ATOM 1977  CG  PRO A 279    7.030  48.019   0.831  1.00 27.27  A C
ATOM 1978  C   PRO A 279    7.575  46.990   3.707  1.00 27.37  A C
ATOM 1979  O   PRO A 279    6.885  45.994   3.438  1.00 27.41  A O
ATOM 1980  N   THR A 280    7.609  47.572   4.905  1.00 27.28  A N
ATOM 1981  CA  THR A 280    6.767  47.155   6.025  1.00 27.53  A C
ATOM 1982  CB  THR A 280    7.343  47.643   7.372  1.00 27.49  A C
ATOM 1983  OG1 THR A 280    7.508  49.062   7.315  1.00 27.40  A O
ATOM 1984  CG2 THR A 280    8.712  47.019   7.654  1.00 27.23  A C
ATOM 1985  C   THR A 280    5.466  47.930   5.773  1.00 27.87  A C
ATOM 1986  O   THR A 280    5.452  48.861   4.959  1.00 27.53  A O
ATOM 1987  N   PHE A 281    4.385  47.570   6.456  1.00 28.47  A N
ATOM 1988  CA  PHE A 281    3.126  48.277   6.266  1.00 29.10  A C
ATOM 1989  CB  PHE A 281    2.035  47.672   7.143  1.00 30.37  A C
ATOM 1990  CG  PHE A 281    1.547  46.363   6.649  1.00 31.79  A C
ATOM 1991  CD1 PHE A 281    2.339  45.231   6.752  1.00 33.01  A C
ATOM 1992  CD2 PHE A 281    0.324  46.260   6.018  1.00 32.62  A C
ATOM 1993  CE1 PHE A 281    1.917  44.011   6.227  1.00 33.47  A C
ATOM 1994  CE2 PHE A 281   -0.102  45.040   5.489  1.00 33.23  A C
ATOM 1995  CZ  PHE A 281    0.696  43.916   5.595  1.00 33.29  A C
ATOM 1996  C   PHE A 281    3.265  49.753   6.573  1.00 28.99  A C
ATOM 1997  O   PHE A 281    2.669  50.599   5.899  1.00 28.64  A O
ATOM 1998  N   GLU A 282    4.069  50.058   7.588  1.00 28.82  A N
ATOM 1999  CA  GLU A 282    4.298  51.444   7.984  1.00 28.61  A C
ATOM 2000  CB  GLU A 282    5.151  51.502   9.258  1.00 29.25  A C
ATOM 2001  CG  GLU A 282    5.550  52.906   9.694  1.00 30.72  A C
ATOM 2002  CD  GLU A 282    6.377  52.909  10.986  1.00 31.82  A C
ATOM 2003  OE1 GLU A 282    7.238  52.018  11.154  1.00 32.10  A O
ATOM 2004  OE2 GLU A 282    6.174  53.808  11.830  1.00 32.22  A O
ATOM 2005  C   GLU A 282    4.994  52.185   6.845  1.00 27.93  A C
ATOM 2006  O   GLU A 282    4.626  53.313   6.526  1.00 27.53  A O
ATOM 2007  N   GLU A 283    5.993  51.550   6.235  1.00 27.27  A N
ATOM 2008  CA  GLU A 283    6.705  52.179   5.123  1.00 27.17  A C
ATOM 2009  CB  GLU A 283    7.913  51.346   4.723  1.00 27.15  A C
ATOM 2010  CG  GLU A 283    9.014  51.390   5.749  1.00 28.08  A C
ATOM 2011  CD  GLU A 283   10.172  50.483   5.398  1.00 28.16  A C
ATOM 2012  OE1 GLU A 283    9.952  49.282   5.196  1.00 28.68  A O
ATOM 2013  OE2 GLU A 283   11.310  50.974   5.328  1.00 29.17  A O
ATOM 2014  C   GLU A 283    5.805  52.408   3.901  1.00 26.64  A C
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FIGURE 2A-37

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ATOM 2015  O   GLU A 283     5.973  53.388   3.170  1.00 26.50  A O
ATOM 2016  N   ILE A 284     4.853  51.507   3.677  1.00 26.15  A N
ATOM 2017  CA  ILE A 284     3.942  51.673   2.553  1.00 25.62  A C
ATOM 2018  CB  ILE A 284     3.055  50.425   2.345  1.00 25.27  A C
ATOM 2019  CG2 ILE A 284     1.925  50.735   1.322  1.00 24.83  A C
ATOM 2020  CG1 ILE A 284     3.917  49.256   1.866  1.00 24.82  A C
ATOM 2021  CD1 ILE A 284     3.135  48.009   1.616  1.00 25.07  A C
ATOM 2022  C   ILE A 284     3.034  52.882   2.796  1.00 25.78  A C
ATOM 2023  O   ILE A 284     2.889  53.739   1.918  1.00 25.89  A O
ATOM 2024  N   GLN A 285     2.440  52.959   3.989  1.00 25.49  A N
ATOM 2025  CA  GLN A 285     1.536  54.061   4.330  1.00 25.62  A C
ATOM 2026  CB  GLN A 285     0.693  53.692   5.565  1.00 25.31  A C
ATOM 2027  CG  GLN A 285    -0.267  52.526   5.295  1.00 24.96  A C
ATOM 2028  CD  GLN A 285    -1.324  52.342   6.374  1.00 25.15  A C
ATOM 2029  OE1 GLN A 285    -1.022  51.911   7.492  1.00 25.27  A O
ATOM 2030  NE2 GLN A 285    -2.570  52.671   6.042  1.00 24.40  A N
ATOM 2031  C   GLN A 285     2.214  55.422   4.541  1.00 25.81  A C
ATOM 2032  O   GLN A 285     1.546  56.460   4.597  1.00 26.16  A O
ATOM 2033  N   ASN A 286     3.534  55.423   4.663  1.00 25.78  A N
ATOM 2034  CA  ASN A 286     4.266  56.676   4.825  1.00 26.03  A C
ATOM 2035  CB  ASN A 286     5.373  56.531   5.882  1.00 25.75  A C
ATOM 2036  CG  ASN A 286     4.862  56.748   7.297  1.00 25.81  A C
ATOM 2037  OD1 ASN A 286     5.442  56.257   8.255  1.00 26.55  A O
ATOM 2038  ND2 ASN A 286     3.785  57.494   7.431  1.00 25.72  A N
ATOM 2039  C   ASN A 286     4.889  57.041   3.482  1.00 26.10  A C
ATOM 2040  O   ASN A 286     5.588  58.043   3.358  1.00 26.33  A O
ATOM 2041  N   HIS A 287     4.636  56.217   2.473  1.00 25.94  A N
ATOM 2042  CA  HIS A 287     5.196  56.476   1.158  1.00 25.88  A C
ATOM 2043  CB  HIS A 287     4.948  55.272   0.242  1.00 24.92  A C
ATOM 2044  CG  HIS A 287     5.673  55.350  -1.062  1.00 23.86  A C
ATOM 2045  CD2 HIS A 287     6.811  54.753  -1.483  1.00 23.35  A C
ATOM 2046  ND1 HIS A 287     5.258  56.161  -2.097  1.00 23.28  A N
ATOM 2047  CE1 HIS A 287     6.110  56.059  -3.101  1.00 23.25  A C
ATOM 2048  NE2 HIS A 287     7.064  55.211  -2.754  1.00 23.22  A N
ATOM 2049  C   HIS A 287     4.582  57.741   0.557  1.00 26.38  A C
ATOM 2050  O   HIS A 287     3.397  58.026   0.752  1.00 26.64  A O
ATOM 2051  N   PRO A 288     5.388  58.534  -0.161  1.00 26.74  A N
ATOM 2052  CD  PRO A 288     6.847  58.410  -0.330  1.00 26.83  A C
ATOM 2053  CA  PRO A 288     4.905  59.765  -0.783  1.00 27.08  A C
ATOM 2054  CB  PRO A 288     6.053  60.143  -1.714  1.00 27.04  A C
ATOM 2055  CG  PRO A 288     7.231  59.770  -0.904  1.00 26.92  A C
ATOM 2056  C   PRO A 288     3.594  59.596  -1.534  1.00 27.37  A C
ATOM 2057  O   PRO A 288     2.713  60.444  -1.442  1.00 27.43  A O
ATOM 2058  N   TRP A 289     3.456  58.497  -2.271  1.00 27.70  A N
ATOM 2059  CA  TRP A 289     2.241  58.273  -3.050  1.00 28.14  A C
ATOM 2060  CB  TRP A 289     2.419  57.064  -3.984  1.00 27.62  A C
ATOM 2061  CG  TRP A 289     1.271  56.888  -4.950  1.00 26.93  A C
ATOM 2062  CD2 TRP A 289     0.164  55.979  -4.821  1.00 26.51  A C
ATOM 2063  CE2 TRP A 289    -0.714  56.231  -5.898  1.00 26.48  A C
ATOM 2064  CE3 TRP A 289    -0.171  54.982  -3.898  1.00 26.39  A C
ATOM 2065  CD1 TRP A 289     1.028  57.625  -6.074  1.00 26.64  A C
ATOM 2066  NE1 TRP A 289    -0.161  57.237  -6.650  1.00 26.64  A N
ATOM 2067  CZ2 TRP A 289    -1.913  55.522  -6.077  1.00 26.18  A C
ATOM 2068  CZ3 TRP A 289    -1.372  54.270  -4.082  1.00 26.53  A C
ATOM 2069  CH2 TRP A 289    -2.221  54.548  -5.161  1.00 26.12  A C
ATOM 2070  C   TRP A 289     0.974  58.086  -2.206  1.00 28.92  A C
```

FIGURE 2A-38

ATOM	2071	O	TRP	A	289	-0.120	58.378	-2.674	1.00	28.75	A	O
ATOM	2072	N	MET	A	290	1.133	57.630	-0.960	1.00	30.06	A	N
ATOM	2073	CA	MET	A	290	0.016	57.361	-0.038	1.00	31.36	A	C
ATOM	2074	CB	MET	A	290	0.432	56.231	0.906	1.00	31.08	A	C
ATOM	2075	CG	MET	A	290	0.583	54.885	0.216	1.00	31.48	A	C
ATOM	2076	SD	MET	A	290	-1.062	54.101	-0.052	1.00	32.05	A	S
ATOM	2077	CE	MET	A	290	-0.939	52.949	1.008	1.00	31.36	A	C
ATOM	2078	C	MET	A	290	-0.544	58.533	0.783	1.00	32.48	A	C
ATOM	2079	O	MET	A	290	-1.513	58.373	1.538	1.00	32.80	A	O
ATOM	2080	N	GLN	A	291	0.041	59.718	0.629	1.00	33.58	A	N
ATOM	2081	CA	GLN	A	291	-0.406	60.899	1.395	1.00	34.40	A	C
ATOM	2082	CB	GLN	A	291	0.749	61.913	1.467	1.00	34.96	A	C
ATOM	2083	CG	GLN	A	291	2.056	61.343	2.048	1.00	36.06	A	C
ATOM	2084	CD	GLN	A	291	1.803	60.403	3.252	1.00	37.05	A	C
ATOM	2085	OE1	GLN	A	291	1.348	60.849	4.313	1.00	37.37	A	O
ATOM	2086	NE2	GLN	A	291	2.079	59.098	3.074	1.00	36.71	A	N
ATOM	2087	C	GLN	A	291	-1.701	61.578	0.897	1.00	34.67	A	C
ATOM	2088	O	GLN	A	291	-2.037	61.488	-0.279	1.00	34.69	A	O
ATOM	2089	N	ASP	A	292	-2.437	62.235	1.796	1.00	34.87	A	N
ATOM	2090	CA	ASP	A	292	-3.686	62.913	1.426	1.00	35.14	A	C
ATOM	2091	CB	ASP	A	292	-3.414	64.020	0.409	1.00	36.16	A	C
ATOM	2092	CG	ASP	A	292	-2.438	65.035	0.922	1.00	37.36	A	C
ATOM	2093	OD1	ASP	A	292	-2.641	65.525	2.064	1.00	38.19	A	O
ATOM	2094	OD2	ASP	A	292	-1.471	65.327	0.188	1.00	38.33	A	O
ATOM	2095	C	ASP	A	292	-4.781	62.003	0.847	1.00	34.78	A	C
ATOM	2096	O	ASP	A	292	-5.415	62.342	-0.157	1.00	34.35	A	O
ATOM	2097	N	VAL	A	293	-5.009	60.863	1.486	1.00	34.32	A	N
ATOM	2098	CA	VAL	A	293	-6.023	59.941	1.016	1.00	33.99	A	C
ATOM	2099	CB	VAL	A	293	-5.897	58.561	1.721	1.00	33.83	A	C
ATOM	2100	CG1	VAL	A	293	-6.102	58.714	3.212	1.00	33.87	A	C
ATOM	2101	CG2	VAL	A	293	-6.901	57.579	1.141	1.00	33.60	A	C
ATOM	2102	C	VAL	A	293	-7.386	60.553	1.298	1.00	33.93	A	C
ATOM	2103	O	VAL	A	293	-7.553	61.305	2.254	1.00	33.93	A	O
ATOM	2104	N	LEU	A	294	-8.349	60.269	0.437	1.00	33.95	A	N
ATOM	2105	CA	LEU	A	294	-9.698	60.780	0.615	1.00	34.08	A	C
ATOM	2106	CB	LEU	A	294	-10.499	60.652	-0.682	1.00	33.63	A	C
ATOM	2107	CG	LEU	A	294	-10.109	61.419	-1.943	1.00	33.58	A	C
ATOM	2108	CD1	LEU	A	294	-11.087	61.068	-3.066	1.00	33.52	A	C
ATOM	2109	CD2	LEU	A	294	-10.131	62.901	-1.673	1.00	33.17	A	C
ATOM	2110	C	LEU	A	294	-10.371	59.912	1.666	1.00	34.38	A	C
ATOM	2111	O	LEU	A	294	-9.915	58.805	1.949	1.00	34.02	A	O
ATOM	2112	N	LEU	A	295	-11.459	60.421	2.235	1.00	34.95	A	N
ATOM	2113	CA	LEU	A	295	-12.235	59.673	3.210	1.00	35.38	A	C
ATOM	2114	CB	LEU	A	295	-13.074	60.619	4.070	1.00	35.64	A	C
ATOM	2115	CG	LEU	A	295	-12.261	61.546	4.976	1.00	36.09	A	C
ATOM	2116	CD1	LEU	A	295	-13.195	62.510	5.720	1.00	36.16	A	C
ATOM	2117	CD2	LEU	A	295	-11.454	60.708	5.949	1.00	36.04	A	C
ATOM	2118	C	LEU	A	295	-13.147	58.764	2.398	1.00	35.61	A	C
ATOM	2119	O	LEU	A	295	-13.438	59.046	1.227	1.00	35.53	A	O
ATOM	2120	N	PRO	A	296	-13.604	57.655	2.997	1.00	35.86	A	N
ATOM	2121	CD	PRO	A	296	-13.249	57.095	4.316	1.00	35.90	A	C
ATOM	2122	CA	PRO	A	296	-14.484	56.747	2.254	1.00	36.07	A	C
ATOM	2123	CB	PRO	A	296	-14.912	55.742	3.315	1.00	35.94	A	C
ATOM	2124	CG	PRO	A	296	-13.674	55.637	4.177	1.00	35.98	A	C
ATOM	2125	C	PRO	A	296	-15.670	57.473	1.633	1.00	36.55	A	C
ATOM	2126	O	PRO	A	296	-15.954	57.324	0.437	1.00	36.17	A	O

FIGURE 2A-39

```
ATOM 2127  N   GLN A 297  -16.351  58.274   2.450  1.00 37.20  A N
ATOM 2128  CA  GLN A 297  -17.525  59.006   1.986  1.00 38.03  A C
ATOM 2129  CB  GLN A 297  -18.211  59.722   3.163  1.00 38.68  A C
ATOM 2130  CG  GLN A 297  -19.616  60.252   2.845  1.00 39.63  A C
ATOM 2131  CD  GLN A 297  -20.515  59.214   2.169  1.00 40.52  A C
ATOM 2132  OE1 GLN A 297  -20.974  58.248   2.793  1.00 40.84  A O
ATOM 2133  NE2 GLN A 297  -20.766  59.411   0.879  1.00 41.21  A N
ATOM 2134  C   GLN A 297  -17.202  59.980   0.849  1.00 37.98  A C
ATOM 2135  O   GLN A 297  -17.992  60.118  -0.078  1.00 38.03  A O
ATOM 2136  N   GLU A 298  -16.053  60.648   0.912  1.00 38.22  A N
ATOM 2137  CA  GLU A 298  -15.659  61.566  -0.164  1.00 38.58  A C
ATOM 2138  CB  GLU A 298  -14.349  62.289   0.148  1.00 39.26  A C
ATOM 2139  CG  GLU A 298  -14.398  63.220   1.307  1.00 40.59  A C
ATOM 2140  CD  GLU A 298  -13.078  63.922   1.519  1.00 41.53  A C
ATOM 2141  OE1 GLU A 298  -12.069  63.240   1.812  1.00 41.65  A O
ATOM 2142  OE2 GLU A 298  -13.052  65.169   1.390  1.00 42.73  A O
ATOM 2143  C   GLU A 298  -15.419  60.721  -1.400  1.00 38.37  A C
ATOM 2144  O   GLU A 298  -15.826  61.077  -2.510  1.00 38.39  A O
ATOM 2145  N   THR A 299  -14.742  59.597  -1.188  1.00 37.86  A N
ATOM 2146  CA  THR A 299  -14.426  58.685  -2.269  1.00 37.55  A C
ATOM 2147  CB  THR A 299  -13.715  57.416  -1.743  1.00 37.21  A C
ATOM 2148  OG1 THR A 299  -12.526  57.793  -1.034  1.00 36.66  A O
ATOM 2149  CG2 THR A 299  -13.353  56.497  -2.890  1.00 36.54  A C
ATOM 2150  C   THR A 299  -15.690  58.263  -3.003  1.00 37.60  A C
ATOM 2151  O   THR A 299  -15.718  58.233  -4.230  1.00 37.42  A O
ATOM 2152  N   ALA A 300  -16.739  57.932  -2.259  1.00 37.62  A N
ATOM 2153  CA  ALA A 300  -17.964  57.505  -2.914  1.00 37.98  A C
ATOM 2154  CB  ALA A 300  -18.932  56.925  -1.897  1.00 37.98  A C
ATOM 2155  C   ALA A 300  -18.608  58.679  -3.653  1.00 38.31  A C
ATOM 2156  O   ALA A 300  -19.032  58.541  -4.798  1.00 38.27  A O
ATOM 2157  N   GLU A 301  -18.656  59.837  -3.002  1.00 38.54  A N
ATOM 2158  CA  GLU A 301  -19.275  61.016  -3.601  1.00 39.05  A C
ATOM 2159  CB  GLU A 301  -19.275  62.178  -2.599  1.00 39.59  A C
ATOM 2160  CG  GLU A 301  -20.325  62.016  -1.497  1.00 40.85  A C
ATOM 2161  CD  GLU A 301  -20.060  62.885  -0.271  1.00 41.55  A C
ATOM 2162  OE1 GLU A 301  -20.840  62.780   0.704  1.00 41.99  A O
ATOM 2163  OE2 GLU A 301  -19.079  63.667  -0.275  1.00 41.81  A O
ATOM 2164  C   GLU A 301  -18.612  61.437  -4.898  1.00 38.92  A C
ATOM 2165  O   GLU A 301  -19.289  61.809  -5.852  1.00 38.90  A O
ATOM 2166  N   ILE A 302  -17.289  61.345  -4.933  1.00 38.77  A N
ATOM 2167  CA  ILE A 302  -16.509  61.726  -6.100  1.00 38.48  A C
ATOM 2168  CB  ILE A 302  -15.091  62.144  -5.691  1.00 38.47  A C
ATOM 2169  CG2 ILE A 302  -14.276  62.506  -6.921  1.00 38.22  A C
ATOM 2170  CG1 ILE A 302  -15.162  63.312  -4.709  1.00 38.37  A C
ATOM 2171  CD1 ILE A 302  -13.824  63.738  -4.178  1.00 38.32  A C
ATOM 2172  C   ILE A 302  -16.354  60.660  -7.174  1.00 38.48  A C
ATOM 2173  O   ILE A 302  -16.344  60.986  -8.359  1.00 38.78  A O
ATOM 2174  N   HIS A 303  -16.243  59.393  -6.776  1.00 38.13  A N
ATOM 2175  CA  HIS A 303  -15.998  58.320  -7.739  1.00 37.74  A C
ATOM 2176  CB  HIS A 303  -14.661  57.648  -7.406  1.00 36.62  A C
ATOM 2177  CG  HIS A 303  -13.473  58.550  -7.536  1.00 35.43  A C
ATOM 2178  CD2 HIS A 303  -12.735  59.189  -6.601  1.00 34.94  A C
ATOM 2179  ND1 HIS A 303  -12.916  58.878  -8.753  1.00 34.94  A N
ATOM 2180  CE1 HIS A 303  -11.884  59.678  -8.561  1.00 34.56  A C
ATOM 2181  NE2 HIS A 303  -11.752  59.883  -7.264  1.00 34.73  A N
ATOM 2182  C   HIS A 303  -17.045  57.225  -7.883  1.00 38.41  A C
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FIGURE 2A-40

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ATOM 2183  O   HIS A 303  -17.066  56.517  -8.901  1.00 38.09  A O
ATOM 2184  N   LEU A 304  -17.905  57.070  -6.881  1.00 39.14  A N
ATOM 2185  CA  LEU A 304  -18.896  56.005  -6.925  1.00 40.20  A C
ATOM 2186  CB  LEU A 304  -18.759  55.152  -5.666  1.00 39.70  A C
ATOM 2187  CG  LEU A 304  -17.344  54.647  -5.380  1.00 39.47  A C
ATOM 2188  CD1 LEU A 304  -17.310  53.968  -4.022  1.00 39.35  A C
ATOM 2189  CD2 LEU A 304  -16.908  53.691  -6.472  1.00 39.04  A C
ATOM 2190  C   LEU A 304  -20.360  56.420  -7.106  1.00 41.19  A C
ATOM 2191  O   LEU A 304  -21.153  55.664  -7.669  1.00 41.18  A O
ATOM 2192  N   HIS A 305  -20.730  57.601  -6.625  1.00 42.42  A N
ATOM 2193  CA  HIS A 305  -22.115  58.046  -6.764  1.00 43.79  A C
ATOM 2194  CB  HIS A 305  -22.369  59.304  -5.926  1.00 44.31  A C
ATOM 2195  CG  HIS A 305  -22.375  59.059  -4.447  1.00 44.92  A C
ATOM 2196  CD2 HIS A 305  -22.537  59.909  -3.402  1.00 44.99  A C
ATOM 2197  ND1 HIS A 305  -22.201  57.805  -3.897  1.00 45.29  A N
ATOM 2198  CE1 HIS A 305  -22.255  57.893  -2.578  1.00 45.20  A C
ATOM 2199  NE2 HIS A 305  -22.457  59.159  -2.253  1.00 45.15  A N
ATOM 2200  C   HIS A 305  -22.411  58.342  -8.233  1.00 44.33  A C
ATOM 2201  O   HIS A 305  -21.555  59.013  -8.863  1.00 44.78  A O
ATOM 2202  OXT HIS A 305  -23.485  57.908  -8.724  1.00 44.44  A O
TER        1   HIS A 305                                      A
HET  2203  O   HOH W   1    5.212  44.355   7.893  1.00 35.40  W O
HET  2204  O   HOH W   2    8.417  38.986   6.811  1.00 32.60  W O
HET  2205  O   HOH W   3  -14.568  38.217   5.927  1.00 21.67  W O
HET  2206  O   HOH W   4   -2.738  38.833   5.268  1.00 22.78  W O
HET  2207  O   HOH W   5    6.255  34.464   8.951  1.00 25.09  W O
HET  2208  O   HOH W   6    2.795  36.994  -8.168  1.00 20.29  W O
HET  2209  O   HOH W   7   -7.740  33.313   2.802  1.00 21.15  W O
HET  2210  O   HOH W   8  -17.206  44.780   8.882  1.00 31.68  W O
HET  2211  O   HOH W   9    0.337  38.925 -11.388  1.00 22.82  W O
HET  2212  O   HOH W  10    8.713  39.589 -15.036  1.00 29.43  W O
HET  2213  O   HOH W  12  -10.989  26.657   6.528  1.00 51.60  W O
HET  2214  O   HOH W  13  -14.596  33.553   5.148  1.00 23.49  W O
HET  2215  O   HOH W  14    5.496  37.378   9.070  1.00 40.82  W O
HET  2216  O   HOH W  15  -10.178  53.351 -17.004  1.00 41.14  W O
HET  2217  O   HOH W  16  -11.373  55.678 -11.919  1.00 26.83  W O
HET  2218  O   HOH W  18   -9.445  42.668 -12.521  1.00 46.50  W O
HET  2219  O   HOH W  19   -3.263  54.539  10.073  1.00 19.58  W O
HET  2220  O   HOH W  20    4.586  47.817   9.766  1.00 23.38  W O
HET  2221  O   HOH W  21  -15.369  36.059   4.383  1.00 26.97  W O
HET  2222  O   HOH W  22    1.949  48.977  10.513  1.00 35.51  W O
HET  2223  O   HOH W  23   -1.967  37.821   0.519  1.00 23.92  W O
HET  2224  O   HOH W  24   -7.240  59.242  -2.232  1.00 26.36  W O
HET  2225  O   HOH W  25   15.115  42.636  -4.103  1.00 28.08  W O
HET  2226  O   HOH W  26   -4.730  58.540 -12.650  1.00 33.46  W O
HET  2227  O   HOH W  27  -12.865  49.765   4.749  1.00 26.81  W O
HET  2228  O   HOH W  28  -10.127  49.485   6.135  1.00 23.82  W O
HET  2229  O   HOH W  29  -10.440  55.854   2.097  1.00 30.94  W O
HET  2230  O   HOH W  30    8.283  54.982   3.094  1.00 22.77  W O
HET  2231  O   HOH W  31   -4.513  54.836 -13.525  1.00 36.98  W O
HET  2232  O   HOH W  32   -5.807  62.589   4.345  1.00 56.33  W O
HET  2233  O   HOH W  33   -2.797  59.486   3.720  1.00 35.39  W O
HET  2234  O   HOH W  34   -7.087  39.196 -10.078  1.00 42.59  W O
HET  2235  O   HOH W  35  -24.718  22.958   4.141  1.00 25.29  W O
HET  2236  O   HOH W  36   15.028  38.185   2.891  1.00 52.12  W O
HET  2237  O   HOH W  37   10.867  45.618  -8.219  1.00 38.83  W O
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FIGURE 2A-41

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HET  2238  O   HOH W  38    3.736  26.370   7.038  1.00 39.08  W O
HET  2239  O   HOH W  39   -9.277  46.706 -16.792  1.00 45.05  W O
HET  2240  O   HOH W  40   -4.278  36.322  -3.784  1.00 29.40  W O
HET  2241  O   HOH W  42   -8.188  51.639  10.340  1.00 37.57  W O
HET  2242  O   HOH W  43    4.308  24.802  -6.902  1.00 55.67  W O
HET  2243  O   HOH W  44    8.947  50.251   9.577  1.00 34.55  W O
HET  2244  O   HOH W  46   15.427  39.450 -12.597  1.00 53.94  W O
HET  2245  O   HOH W  48    9.455  24.154   1.642  1.00 37.76  W O
HET  2246  O   HOH W  49  -29.401  30.984  -6.964  1.00 39.78  W O
HET  2247  O   HOH W  50   -8.109  50.401 -18.412  1.00 40.63  W O
HET  2248  O   HOH W  51  -30.954  30.086  -3.494  1.00 31.99  W O
HET  2249  O   HOH W  52   -0.586  35.769  -0.747  1.00 34.60  W O
HET  2250  O   HOH W  53  -24.284  48.859   3.821  1.00 71.39  W O
HET  2251  O   HOH W  55    8.047  65.651 -13.476  1.00 54.19  W O
HET  2252  O   HOH W  56  -18.470  16.700   3.474  1.00 48.72  W O
HET  2253  O   HOH W  57   -5.322  26.757   3.066  1.00 54.14  W O
HET  2254  O   HOH W  58    5.025  63.559  -3.416  1.00 56.14  W O
HET  2255  O   HOH W  59  -24.745  56.608   8.909  1.00 53.88  W O
HET  2256  O   HOH W  60   -5.993  61.575  -2.626  1.00 32.62  W O
HET  2257  O   HOH W  61   -1.987  34.307  15.886  1.00 36.44  W O
HET  2258  O   HOH W  63   10.978  43.204  -8.974  1.00 23.08  W O
HET  2259  O   HOH W  64   -1.608  37.699   3.126  1.00 22.94  W O
HET  2260  O   HOH W  65    8.616  35.812   2.340  1.00 24.46  W O
HET  2261  O   HOH W  66   -7.639  27.345   0.580  1.00 45.82  W O
HET  2262  O   HOH W  67   -6.912  63.760  -4.055  1.00 47.64  W O
HET  2263  O   HOH W  69    1.745  36.696  -1.868  1.00 26.81  W O
HET  2264  O   HOH W  71  -17.429  24.985  -4.905  1.00 35.04  W O
HET  2265  O   HOH W  72  -19.600  24.497  -3.015  1.00 29.29  W O
HET  2266  O   HOH W  73  -24.271  51.032   2.229  1.00 38.47  W O
HET  2267  O   HOH W  74   -0.895  62.286  -2.569  1.00 39.95  W O
HET  2268  O   HOH W  76    9.873  61.551 -15.061  1.00 37.54  W O
HET  2269  O   HOH W  77  -13.578  57.531 -11.018  1.00 39.01  W O
HET  2270  O   HOH W  78   10.121  52.616 -10.455  1.00 44.06  W O
HET  2271  O   HOH W  79    7.327  43.491   4.160  1.00 22.80  W O
HET  2272  O   HOH W  80  -15.673  58.533   5.455  1.00 37.18  W O
HET  2273  O   HOH W  83  -11.963  33.730  -2.896  1.00 21.54  W O
HET  2274  O   HOH W  84  -18.124  23.005  -0.952  1.00 25.45  W O
HET  2275  O   HOH W  85    1.314  51.350   9.331  1.00 33.30  W O
HET  2276  O   HOH W  86    0.631  27.781  -5.580  1.00 29.86  W O
HET  2277  O   HOH W  87    0.847  36.241   3.337  1.00 18.60  W O
HET  2278  O   HOH W  88   10.456  38.307   5.314  1.00 27.40  W O
HET  2279  O   HOH W  89   12.095  47.498   4.202  1.00 44.68  W O
HET  2280  O   HOH W  90   -5.824  49.207  11.039  1.00 26.73  W O
HET  2281  O   HOH W  91    0.625  34.446   1.430  1.00 31.58  W O
HET  2282  O   HOH W  92  -23.548  29.347 -10.396  1.00 29.01  W O
HET  2283  O   HOH W  93  -19.510  41.574  -7.708  1.00 27.71  W O
HET  2284  O   HOH W  94    5.935  32.764  15.692  1.00 30.76  W O
HET  2285  O   HOH W  95    3.716  37.237  15.437  1.00 63.54  W O
HET  2286  O   HOH W  96    9.156  39.155 -17.589  1.00 34.60  W O
HET  2287  O   HOH W  97  -19.458  31.825  -9.046  1.00 30.22  W O
HET  2288  O   HOH W  98  -10.749  29.515  -1.814  1.00 48.58  W O
HET  2289  O   HOH W  99   -3.021  29.184   1.922  1.00 28.07  W O
HET  2290  O   HOH W 100  -10.659  32.330  17.462  1.00 41.13  W O
HET  2291  O   HOH W 101   -6.124  60.850  -9.621  1.00 33.81  W O
HET  2292  O   HOH W 102  -14.593  49.718   6.791  1.00 38.42  W O
HET  2293  O   HOH W 103  -20.957  43.101 -10.957  1.00 32.50  W O
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FIGURE 2A-42

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HET  2294  O   HOH W 104   -3.213  32.059  -9.993  1.00 33.63  W O
HET  2295  O   HOH W 105   -4.224  30.052  -8.162  1.00 37.86  W O
HET  2296  O   HOH W 106   -2.430  34.513  -2.817  1.00 29.57  W O
HET  2297  O   HOH W 107  -19.920  49.497   4.394  1.00 39.12  W O
HET  2298  O   HOH W 108   11.612  24.185   3.333  1.00 46.30  W O
HET  2299  O   HOH W 109  -35.236  30.646   2.831  1.00 49.80  W O
HET  2300  O   HOH W 110   11.157  51.039  -5.972  1.00 45.82  W O
HET  2301  O   HOH W 111  -25.455  28.662  16.250  1.00 56.18  W O
HET  2302  O   HOH W 112   -4.133  62.224  -7.121  1.00 37.52  W O
HET  2303  O   HOH W 113    3.358  29.072 -14.953  1.00 40.02  W O
HET  2304  O   HOH W 114    5.238  56.384  11.178  1.00 38.89  W O
HET  2305  O   HOH W 115   -2.136  27.965  -5.144  1.00 44.79  W O
HET  2306  O   HOH W 116  -25.651  44.713  -3.228  1.00 39.36  W O
HET  2307  O   HOH W 117   -2.725  28.375  11.139  1.00 37.27  W O
HET  2308  O   HOH W 118    1.582  32.255  15.957  1.00 33.46  W O
HET  2309  O   HOH W 119  -22.441  42.820  -7.377  1.00 34.26  W O
HET  2310  O   HOH W 120    4.807  43.441 -15.921  1.00 30.97  W O
HET  2311  O   HOH W 121   -8.937  31.920  -0.415  1.00 32.42  W O
HET  2312  O   HOH W 122  -19.155  35.814  -8.083  1.00 51.00  W O
HET  2313  O   HOH W 123  -14.515  23.686  -2.506  1.00 61.58  W O
HET  2314  O   HOH W 124  -15.546  22.895  -5.055  1.00 50.13  W O
HET  2315  O   HOH W 125  -24.773  42.675   7.542  1.00 40.80  W O
HET  2316  O   HOH W 126   10.163  43.072   3.813  1.00 32.95  W O
HET  2317  O   HOH W 127   10.498  46.597 -12.786  1.00 42.87  W O
HET  2318  O   HOH W 128  -17.057  49.685   7.396  1.00 55.77  W O
HET  2319  O   HOH W 129  -28.205  28.717   2.329  1.00 47.88  W O
HET  2320  O   HOH W 130    9.468  57.122 -13.804  1.00 44.49  W O
HET  2321  O   HOH W 131    0.835  23.801   0.084  1.00 41.17  W O
HET  2322  O   HOH W 132  -31.146  42.444   1.157  1.00 42.73  W O
HET  2323  O   HOH W 133  -25.498  43.162  -0.886  1.00 28.92  W O
HET  2324  O   HOH W 134   -9.937  48.101   8.915  1.00 30.08  W O
HET  2325  O   HOH W 135   13.602  43.283  -7.503  1.00 35.13  W O
HET  2326  O   HOH W 136  -20.971  29.116  -9.174  1.00 29.52  W O
HET  2327  O   HOH W 137    6.206  29.957  15.120  1.00 39.19  W O
HET  2328  O   HOH W 138  -21.363  33.450  -9.815  1.00 47.38  W O
HET  2329  O   HOH W 140    1.498  27.566   9.993  1.00 33.91  W O
HET  2330  O   HOH W 141   13.608  30.494   2.649  1.00 35.06  W O
HET  2331  O   HOH W 142  -22.040  37.657  -7.186  1.00 31.45  W O
HET  2332  O   HOH W 143    0.079  29.402  11.248  1.00 35.29  W O
HET  2333  O   HOH W 144  -12.176  29.360  -6.291  1.00 43.13  W O
HET  2334  O   HOH W 145   11.867  51.888  -8.588  1.00 35.43  W O
HET  2335  O   HOH W 146  -22.596  58.234   8.668  1.00 43.78  W O
HET  2336  O   HOH W 147  -13.978  43.051  12.898  1.00 42.64  W O
HET  2337  O   HOH W 148   13.528  48.338   2.159  1.00 49.51  W O
HET  2338  O   HOH W 149   10.933  34.654   3.136  1.00 33.39  W O
HET  2339  O   HOH W 150   17.064  37.420   4.532  1.00 44.57  W O
HET  2340  O   HOH W 151  -13.621  28.198   2.952  1.00 41.29  W O
HET  2341  O   HOH W 152   -2.858  26.020   3.013  1.00 40.24  W O
HET  2342  O   HOH W 153  -31.440  37.873  -0.079  1.00 36.14  W O
HET  2343  O   HOH W 154  -25.576  57.215  11.651  1.00 43.17  W O
HET  2344  O   HOH W 155   -1.017  62.578   4.341  1.00 44.81  W O
HET  2380  O   HOH W 156  -14.113  31.287   2.674  1.00 40.40  W O
HET  2381  O   HOH W 157  -16.214  38.738  -9.405  1.00 37.08  W O
HET  2382  O   HOH W 158   -9.097  53.539   9.066  1.00 35.07  W O
HET  2383  O   HOH W 159    7.055  43.042   6.394  1.00 38.28  W O
HET  2384  O   HOH W 160  -19.558  39.109  -7.269  1.00 38.32  W O
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FIGURE 2A-43

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HET  2385  O   HOH W 161   -2.684  56.549 -13.288  1.00 37.13  W O
HET  2386  O   HOH W 162    0.031  27.041   7.341  1.00 40.61  W O
HET  2387  O   HOH W 163    2.724  62.517 -12.063  1.00 40.62  W O
HET  2388  O   HOH W 164    3.494  33.338  16.949  1.00 42.73  W O
HET  2389  O   HOH W 165   -7.905  47.934 -18.746  1.00 42.41  W O
HET  2345  C1  STO Z   1  -17.190  35.048   1.581  1.00 24.39  Z C
HET  2346  C2  STO Z   1  -16.210  33.972   1.415  1.00 24.28  Z C
HET  2347  C3  STO Z   1  -15.849  33.457   0.091  1.00 24.49  Z C
HET  2348  C4  STO Z   1  -16.482  34.008  -1.111  1.00 24.37  Z C
HET  2349  C5  STO Z   1  -17.474  35.093  -0.955  1.00 24.69  Z C
HET  2350  N1  STO Z   1  -18.229  35.797  -1.944  1.00 24.92  Z N
HET  2351  C6  STO Z   1  -18.944  36.794  -1.236  1.00 24.88  Z C
HET  2352  C7  STO Z   1  -19.809  37.848  -1.790  1.00 25.03  Z C
HET  2353  N2  STO Z   1  -20.055  38.130  -3.130  1.00 25.52  Z N
HET  2354  C8  STO Z   1  -20.928  39.278  -3.194  1.00 25.75  Z C
HET  2355  C9  STO Z   1  -21.519  39.987  -4.363  1.00 26.03  Z C
HET  2356  C10 STO Z   1  -22.416  41.141  -4.128  1.00 25.71  Z C
HET  2357  C11 STO Z   1  -22.719  41.583  -2.747  1.00 25.67  Z C
HET  2358  C12 STO Z   1  -22.123  40.872  -1.580  1.00 25.77  Z C
HET  2359  C13 STO Z   1  -21.230  39.723  -1.826  1.00 25.50  Z C
HET  2360  C14 STO Z   1  -20.516  38.781  -0.927  1.00 25.10  Z C
HET  2361  C15 STO Z   1  -20.328  38.658   0.532  1.00 24.91  Z C
HET  2362  C16 STO Z   1  -20.835  39.482   1.605  1.00 25.07  Z C
HET  2363  N3  STO Z   1  -20.262  39.086   2.768  1.00 24.96  Z N
HET  2364  C17 STO Z   1  -19.450  37.859   2.607  1.00 24.63  Z C
HET  2365  C18 STO Z   1  -19.471  37.663   1.109  1.00 24.72  Z C
HET  2366  C19 STO Z   1  -18.770  36.707   0.205  1.00 24.66  Z C
HET  2367  C20 STO Z   1  -17.810  35.606   0.386  1.00 24.60  Z C
HET  2368  C21 STO Z   1  -18.301  35.477  -3.459  1.00 25.27  Z C
HET  2369  C22 STO Z   1  -16.936  35.811  -4.228  1.00 24.98  Z C
HET  2370  C23 STO Z   1  -17.112  37.004  -5.207  1.00 25.27  Z C
HET  2371  C24 STO Z   1  -17.971  38.083  -4.545  1.00 25.64  Z C
HET  2372  C25 STO Z   1  -19.395  37.530  -4.245  1.00 25.43  Z C
HET  2373  O1  STO Z   1  -19.428  36.151  -4.080  1.00 25.69  Z O
HET  2374  O2  STO Z   1  -21.651  40.389   1.455  1.00 25.66  Z O
HET  2375  N4  STO Z   1  -15.881  37.639  -5.707  1.00 25.27  Z N
HET  2376  C26 STO Z   1  -15.338  36.684  -6.689  1.00 24.85  Z C
HET  2377  O3  STO Z   1  -15.935  36.196  -3.283  1.00 24.52  Z O
HET  2378  C27 STO Z   1  -14.670  35.524  -3.447  1.00 23.53  Z C
HET  2379  C28 STO Z   1  -18.633  33.986  -3.730  1.00 25.05  Z C
END
```

FIGURE 3A-1

ATOM	Type	Resid	#	X	Y	Z	Occ	B	
ATOM	1	CB	PRO A	33	-33.999	26.506	14.294	1.00	75.23	A C
ATOM	2	CG	PRO A	33	-33.664	27.271	15.584	1.00	75.32	A C
ATOM	3	C	PRO A	33	-32.162	27.277	12.754	1.00	75.02	A C
ATOM	4	O	PRO A	33	-32.466	28.463	12.909	1.00	75.11	A O
ATOM	5	N	PRO A	33	-31.694	26.166	14.927	1.00	75.33	A N
ATOM	6	CD	PRO A	33	-32.423	26.554	16.149	1.00	75.36	A C
ATOM	7	CA	PRO A	33	-32.605	26.210	13.756	1.00	75.18	A C
ATOM	8	N	LEU A	34	-31.441	26.843	11.726	1.00	74.67	A N
ATOM	9	CA	LEU A	34	-30.935	27.742	10.694	1.00	74.04	A C
ATOM	10	CB	LEU A	34	-29.765	27.071	9.965	1.00	73.85	A C
ATOM	11	CG	LEU A	34	-28.918	27.856	8.960	1.00	73.74	A C
ATOM	12	CD1	LEU A	34	-27.794	26.953	8.493	1.00	73.70	A C
ATOM	13	CD2	LEU A	34	-29.749	28.328	7.771	1.00	73.63	A C
ATOM	14	C	LEU A	34	-32.032	28.111	9.693	1.00	73.63	A C
ATOM	15	O	LEU A	34	-32.254	29.289	9.401	1.00	73.54	A O
ATOM	16	N	GLU A	35	-32.708	27.093	9.172	1.00	72.96	A N
ATOM	17	CA	GLU A	35	-33.776	27.276	8.193	1.00	72.25	A C
ATOM	18	CB	GLU A	35	-34.377	25.917	7.818	1.00	72.86	A C
ATOM	19	CG	GLU A	35	-33.953	24.775	8.736	1.00	73.58	A C
ATOM	20	CD	GLU A	35	-32.701	24.069	8.245	1.00	74.04	A C
ATOM	21	OE1	GLU A	35	-32.040	23.386	9.060	1.00	74.15	A O
ATOM	22	OE2	GLU A	35	-32.387	24.187	7.039	1.00	74.29	A O
ATOM	23	C	GLU A	35	-34.895	28.206	8.661	1.00	71.32	A C
ATOM	24	O	GLU A	35	-35.705	28.663	7.852	1.00	71.37	A O
ATOM	25	N	SER A	36	-34.942	28.488	9.959	1.00	69.96	A N
ATOM	26	CA	SER A	36	-35.986	29.354	10.498	1.00	68.45	A C
ATOM	27	CB	SER A	36	-36.502	28.794	11.829	1.00	68.80	A C
ATOM	28	OG	SER A	36	-35.470	28.736	12.800	1.00	69.17	A O
ATOM	29	C	SER A	36	-35.547	30.802	10.692	1.00	66.95	A C
ATOM	30	O	SER A	36	-36.359	31.719	10.576	1.00	66.85	A O
ATOM	31	N	GLN A	37	-34.268	31.011	10.984	1.00	65.11	A N
ATOM	32	CA	GLN A	37	-33.758	32.361	11.204	1.00	63.22	A C
ATOM	33	CB	GLN A	37	-32.515	32.317	12.082	1.00	62.94	A C
ATOM	34	CG	GLN A	37	-32.804	32.183	13.549	1.00	62.87	A C
ATOM	35	CD	GLN A	37	-31.540	32.174	14.365	1.00	62.68	A C
ATOM	36	OE1	GLN A	37	-30.747	31.236	14.287	1.00	62.67	A O
ATOM	37	NE2	GLN A	37	-31.335	33.226	15.146	1.00	62.61	A N
ATOM	38	C	GLN A	37	-33.425	33.139	9.940	1.00	61.96	A C
ATOM	39	O	GLN A	37	-33.609	34.356	9.888	1.00	61.76	A O
ATOM	40	N	TYR A	38	-32.932	32.440	8.926	1.00	60.43	A N
ATOM	41	CA	TYR A	38	-32.551	33.090	7.683	1.00	58.96	A C
ATOM	42	CB	TYR A	38	-31.068	32.839	7.414	1.00	58.13	A C
ATOM	43	CG	TYR A	38	-30.183	33.325	8.533	1.00	57.09	A C
ATOM	44	CD1	TYR A	38	-29.956	34.685	8.724	1.00	56.68	A C
ATOM	45	CE1	TYR A	38	-29.188	35.141	9.784	1.00	56.43	A C
ATOM	46	CD2	TYR A	38	-29.615	32.429	9.434	1.00	56.56	A C
ATOM	47	CE2	TYR A	38	-28.848	32.875	10.500	1.00	56.35	A C
ATOM	48	CZ	TYR A	38	-28.639	34.231	10.670	1.00	56.23	A C
ATOM	49	OH	TYR A	38	-27.886	34.680	11.728	1.00	56.16	A O
ATOM	50	C	TYR A	38	-33.374	32.628	6.496	1.00	58.44	A C
ATOM	51	O	TYR A	38	-33.705	31.449	6.371	1.00	58.74	A O
ATOM	52	N	GLN A	39	-33.702	33.574	5.625	1.00	57.37	A N
ATOM	53	CA	GLN A	39	-34.474	33.282	4.433	1.00	56.33	A C

FIGURE 3A-2

```
ATOM    54  CB  GLN A  39  -35.581  34.318   4.266  1.00 57.05  A C
ATOM    55  CG  GLN A  39  -36.462  34.092   3.062  1.00 58.58  A C
ATOM    56  CD  GLN A  39  -37.655  35.023   3.045  1.00 60.00  A C
ATOM    57  OE1 GLN A  39  -37.511  36.239   3.190  1.00 60.34  A O
ATOM    58  NE2 GLN A  39  -38.847  34.456   2.865  1.00 60.77  A N
ATOM    59  C   GLN A  39  -33.527  33.310   3.240  1.00 55.10  A C
ATOM    60  O   GLN A  39  -33.184  34.376   2.727  1.00 55.30  A O
ATOM    61  N   VAL A  40  -33.103  32.124   2.815  1.00 53.39  A N
ATOM    62  CA  VAL A  40  -32.176  31.974   1.698  1.00 51.82  A C
ATOM    63  CB  VAL A  40  -31.921  30.490   1.407  1.00 51.51  A C
ATOM    64  CG1 VAL A  40  -31.059  30.340   0.168  1.00 51.49  A C
ATOM    65  CG2 VAL A  40  -31.244  29.848   2.604  1.00 51.76  A C
ATOM    66  C   VAL A  40  -32.596  32.655   0.397  1.00 50.93  A C
ATOM    67  O   VAL A  40  -33.767  32.651   0.022  1.00 50.89  A O
ATOM    68  N   GLY A  41  -31.615  33.233  -0.286  1.00 49.85  A N
ATOM    69  CA  GLY A  41  -31.869  33.912  -1.540  1.00 48.27  A C
ATOM    70  C   GLY A  41  -31.135  33.239  -2.683  1.00 47.46  A C
ATOM    71  O   GLY A  41  -30.822  32.049  -2.601  1.00 47.43  A O
ATOM    72  N   PRO A  42  -30.830  33.976  -3.761  1.00 46.67  A N
ATOM    73  CD  PRO A  42  -31.080  35.418  -3.942  1.00 46.50  A C
ATOM    74  CA  PRO A  42  -30.128  33.421  -4.920  1.00 46.27  A C
ATOM    75  CB  PRO A  42  -30.266  34.527  -5.957  1.00 46.12  A C
ATOM    76  CG  PRO A  42  -30.179  35.759  -5.114  1.00 46.20  A C
ATOM    77  C   PRO A  42  -28.669  33.070  -4.648  1.00 46.07  A C
ATOM    78  O   PRO A  42  -28.038  33.631  -3.748  1.00 46.12  A O
ATOM    79  N   LEU A  43  -28.140  32.136  -5.431  1.00 45.40  A N
ATOM    80  CA  LEU A  43  -26.749  31.727  -5.292  1.00 44.67  A C
ATOM    81  CB  LEU A  43  -26.469  30.500  -6.164  1.00 44.62  A C
ATOM    82  CG  LEU A  43  -25.032  29.973  -6.229  1.00 44.52  A C
ATOM    83  CD1 LEU A  43  -24.647  29.350  -4.896  1.00 44.26  A C
ATOM    84  CD2 LEU A  43  -24.920  28.943  -7.340  1.00 44.52  A C
ATOM    85  C   LEU A  43  -25.880  32.892  -5.753  1.00 44.11  A C
ATOM    86  O   LEU A  43  -26.047  33.395  -6.861  1.00 43.90  A O
ATOM    87  N   LEU A  44  -24.962  33.330  -4.901  1.00 43.73  A N
ATOM    88  CA  LEU A  44  -24.083  34.432  -5.258  1.00 43.33  A C
ATOM    89  CB  LEU A  44  -23.624  35.173  -4.003  1.00 43.20  A C
ATOM    90  CG  LEU A  44  -24.663  36.117  -3.395  1.00 43.42  A C
ATOM    91  CD1 LEU A  44  -24.155  36.666  -2.081  1.00 43.63  A C
ATOM    92  CD2 LEU A  44  -24.947  37.254  -4.363  1.00 43.17  A C
ATOM    93  C   LEU A  44  -22.880  33.940  -6.046  1.00 43.15  A C
ATOM    94  O   LEU A  44  -22.391  34.632  -6.936  1.00 42.93  A O
ATOM    95  N   GLY A  45  -22.419  32.736  -5.722  1.00 43.20  A N
ATOM    96  CA  GLY A  45  -21.272  32.161  -6.403  1.00 43.13  A C
ATOM    97  C   GLY A  45  -20.706  31.002  -5.612  1.00 43.57  A C
ATOM    98  O   GLY A  45  -21.119  30.763  -4.479  1.00 43.20  A O
ATOM    99  N   SER A  46  -19.762  30.275  -6.196  1.00 44.50  A N
ATOM   100  CA  SER A  46  -19.167  29.140  -5.505  1.00 46.13  A C
ATOM   101  CB  SER A  46  -20.056  27.910  -5.645  1.00 46.12  A C
ATOM   102  OG  SER A  46  -20.023  27.428  -6.978  1.00 46.67  A O
ATOM   103  C   SER A  46  -17.788  28.797  -6.040  1.00 47.45  A C
ATOM   104  O   SER A  46  -17.313  29.393  -7.007  1.00 47.34  A O
ATOM   105  N   GLY A  47  -17.157  27.817  -5.401  1.00 49.10  A N
ATOM   106  CA  GLY A  47  -15.834  27.380  -5.808  1.00 51.09  A C
ATOM   107  C   GLY A  47  -15.326  26.306  -4.868  1.00 52.48  A C
ATOM   108  O   GLY A  47  -16.122  25.591  -4.253  1.00 53.09  A O
ATOM   109  N   GLY A  48  -14.007  26.180  -4.753  1.00 53.41  A N
```

FIGURE 3A-3

```
ATOM  110  CA  GLY A  48  -13.449  25.183  -3.856  1.00 54.40  A C
ATOM  111  C   GLY A  48  -13.762  25.572  -2.422  1.00 55.14  A C
ATOM  112  O   GLY A  48  -13.864  24.723  -1.527  1.00 55.47  A O
ATOM  113  N   PHE A  49  -13.928  26.879  -2.224  1.00 55.12  A N
ATOM  114  CA  PHE A  49  -14.236  27.480  -0.929  1.00 54.83  A C
ATOM  115  CB  PHE A  49  -13.978  28.978  -1.013  1.00 56.58  A C
ATOM  116  CG  PHE A  49  -14.627  29.623  -2.203  1.00 58.74  A C
ATOM  117  CD1 PHE A  49  -13.988  29.632  -3.444  1.00 59.44  A C
ATOM  118  CD2 PHE A  49  -15.906  30.171  -2.100  1.00 59.34  A C
ATOM  119  CE1 PHE A  49  -14.614  30.179  -4.568  1.00 59.87  A C
ATOM  120  CE2 PHE A  49  -16.539  30.716  -3.213  1.00 59.73  A C
ATOM  121  CZ  PHE A  49  -15.893  30.722  -4.452  1.00 60.03  A C
ATOM  122  C   PHE A  49  -15.690  27.254  -0.489  1.00 53.80  A C
ATOM  123  O   PHE A  49  -16.099  27.716   0.579  1.00 53.78  A O
ATOM  124  N   GLY A  50  -16.469  26.559  -1.317  1.00 52.37  A N
ATOM  125  CA  GLY A  50  -17.860  26.299  -0.983  1.00 49.97  A C
ATOM  126  C   GLY A  50  -18.831  27.117  -1.814  1.00 48.12  A C
ATOM  127  O   GLY A  50  -18.455  27.673  -2.850  1.00 48.47  A O
ATOM  128  N   SER A  51  -20.081  27.189  -1.363  1.00 45.87  A N
ATOM  129  CA  SER A  51  -21.117  27.943  -2.064  1.00 43.41  A C
ATOM  130  CB  SER A  51  -22.274  27.019  -2.450  1.00 43.40  A C
ATOM  131  OG  SER A  51  -21.832  25.941  -3.257  1.00 43.30  A O
ATOM  132  C   SER A  51  -21.642  29.067  -1.178  1.00 41.96  A C
ATOM  133  O   SER A  51  -21.821  28.882   0.023  1.00 41.41  A O
ATOM  134  N   VAL A  52  -21.895  30.227  -1.776  1.00 40.70  A N
ATOM  135  CA  VAL A  52  -22.392  31.377  -1.030  1.00 39.61  A C
ATOM  136  CB  VAL A  52  -21.361  32.523  -1.055  1.00 39.33  A C
ATOM  137  CG1 VAL A  52  -21.878  33.722  -0.274  1.00 38.19  A C
ATOM  138  CG2 VAL A  52  -20.047  32.036  -0.473  1.00 39.20  A C
ATOM  139  C   VAL A  52  -23.716  31.882  -1.594  1.00 39.57  A C
ATOM  140  O   VAL A  52  -23.826  32.151  -2.791  1.00 39.11  A O
ATOM  141  N   TYR A  53  -24.716  32.004  -0.719  1.00 39.44  A N
ATOM  142  CA  TYR A  53  -26.047  32.469  -1.104  1.00 39.33  A C
ATOM  143  CB  TYR A  53  -27.127  31.470  -0.671  1.00 38.30  A C
ATOM  144  CG  TYR A  53  -27.014  30.088  -1.266  1.00 37.39  A C
ATOM  145  CD1 TYR A  53  -26.088  29.172  -0.778  1.00 37.03  A C
ATOM  146  CE1 TYR A  53  -25.992  27.895  -1.315  1.00 36.75  A C
ATOM  147  CD2 TYR A  53  -27.845  29.693  -2.309  1.00 36.66  A C
ATOM  148  CE2 TYR A  53  -27.758  28.421  -2.853  1.00 36.79  A C
ATOM  149  CZ  TYR A  53  -26.829  27.527  -2.352  1.00 37.05  A C
ATOM  150  OH  TYR A  53  -26.728  26.268  -2.893  1.00 37.68  A O
ATOM  151  C   TYR A  53  -26.386  33.803  -0.463  1.00 40.05  A C
ATOM  152  O   TYR A  53  -25.908  34.118   0.627  1.00 40.15  A O
ATOM  153  N   SER A  54  -27.222  34.583  -1.143  1.00 40.85  A N
ATOM  154  CA  SER A  54  -27.657  35.865  -0.612  1.00 41.51  A C
ATOM  155  CB  SER A  54  -28.249  36.741  -1.717  1.00 41.66  A C
ATOM  156  OG  SER A  54  -28.705  37.982  -1.194  1.00 42.30  A O
ATOM  157  C   SER A  54  -28.737  35.485   0.379  1.00 42.06  A C
ATOM  158  O   SER A  54  -29.268  34.382   0.308  1.00 42.10  A O
ATOM  159  N   GLY A  55  -29.065  36.376   1.304  1.00 43.11  A N
ATOM  160  CA  GLY A  55  -30.088  36.040   2.274  1.00 44.54  A C
ATOM  161  C   GLY A  55  -30.434  37.164   3.221  1.00 45.80  A C
ATOM  162  O   GLY A  55  -29.784  38.210   3.241  1.00 45.87  A O
ATOM  163  N   ILE A  56  -31.476  36.947   4.010  1.00 46.96  A N
ATOM  164  CA  ILE A  56  -31.912  37.948   4.965  1.00 48.27  A C
ATOM  165  CB  ILE A  56  -33.143  38.714   4.435  1.00 48.57  A C
```

FIGURE 3A-4

```
ATOM  166  CG2 ILE A  56  -32.752  39.546   3.221  1.00 48.29  A C
ATOM  167  CG1 ILE A  56  -34.250  37.728   4.055  1.00 49.41  A C
ATOM  168  CD1 ILE A  56  -35.501  38.391   3.486  1.00 50.04  A C
ATOM  169  C   ILE A  56  -32.246  37.293   6.297  1.00 48.63  A C
ATOM  170  O   ILE A  56  -32.825  36.209   6.344  1.00 48.75  A O
ATOM  171  N   ARG A  57  -31.853  37.949   7.380  1.00 49.30  A N
ATOM  172  CA  ARG A  57  -32.120  37.436   8.715  1.00 50.11  A C
ATOM  173  CB  ARG A  57  -31.178  38.097   9.724  1.00 49.64  A C
ATOM  174  CG  ARG A  57  -31.349  37.614  11.147  1.00 48.93  A C
ATOM  175  CD  ARG A  57  -30.877  38.671  12.128  1.00 48.83  A C
ATOM  176  NE  ARG A  57  -29.448  38.618  12.420  1.00 48.06  A N
ATOM  177  CZ  ARG A  57  -28.769  39.623  12.967  1.00 47.78  A C
ATOM  178  NH1 ARG A  57  -29.391  40.756  13.268  1.00 46.81  A N
ATOM  179  NH2 ARG A  57  -27.474  39.494  13.226  1.00 47.75  A N
ATOM  180  C   ARG A  57  -33.568  37.786   9.038  1.00 50.91  A C
ATOM  181  O   ARG A  57  -33.874  38.938   9.344  1.00 51.41  A O
ATOM  182  N   VAL A  58  -34.452  36.793   8.953  1.00 51.65  A N
ATOM  183  CA  VAL A  58  -35.878  36.986   9.219  1.00 52.14  A C
ATOM  184  CB  VAL A  58  -36.577  35.643   9.494  1.00 52.06  A C
ATOM  185  CG1 VAL A  58  -38.074  35.851   9.598  1.00 52.23  A C
ATOM  186  CG2 VAL A  58  -36.252  34.653   8.391  1.00 52.38  A C
ATOM  187  C   VAL A  58  -36.097  37.900  10.418  1.00 52.54  A C
ATOM  188  O   VAL A  58  -36.973  38.765  10.407  1.00 52.57  A O
ATOM  189  N   SER A  59  -35.282  37.695  11.446  1.00 52.98  A N
ATOM  190  CA  SER A  59  -35.338  38.482  12.670  1.00 53.29  A C
ATOM  191  CB  SER A  59  -34.070  38.226  13.496  1.00 53.65  A C
ATOM  192  OG  SER A  59  -33.918  39.186  14.529  1.00 54.30  A O
ATOM  193  C   SER A  59  -35.504  39.987  12.442  1.00 53.30  A C
ATOM  194  O   SER A  59  -36.217  40.650  13.194  1.00 53.24  A O
ATOM  195  N   ASP A  60  -34.855  40.530  11.413  1.00 53.36  A N
ATOM  196  CA  ASP A  60  -34.948  41.966  11.150  1.00 53.25  A C
ATOM  197  CB  ASP A  60  -34.017  42.729  12.106  1.00 53.02  A C
ATOM  198  CG  ASP A  60  -32.554  42.357  11.928  1.00 53.13  A C
ATOM  199  OD1 ASP A  60  -32.224  41.156  11.990  1.00 53.20  A O
ATOM  200  OD2 ASP A  60  -31.726  43.268  11.730  1.00 53.50  A O
ATOM  201  C   ASP A  60  -34.659  42.395   9.710  1.00 53.18  A C
ATOM  202  O   ASP A  60  -34.388  43.570   9.456  1.00 53.33  A O
ATOM  203  N   ASN A  61  -34.724  41.452   8.774  1.00 53.02  A N
ATOM  204  CA  ASN A  61  -34.472  41.741   7.358  1.00 52.86  A C
ATOM  205  CB  ASN A  61  -35.407  42.844   6.859  1.00 54.15  A C
ATOM  206  CG  ASN A  61  -36.861  42.504   7.064  1.00 55.77  A C
ATOM  207  OD1 ASN A  61  -37.349  41.485   6.567  1.00 56.25  A O
ATOM  208  ND2 ASN A  61  -37.569  43.356   7.804  1.00 56.12  A N
ATOM  209  C   ASN A  61  -33.033  42.159   7.068  1.00 51.79  A C
ATOM  210  O   ASN A  61  -32.734  42.653   5.979  1.00 51.86  A O
ATOM  211  N   LEU A  62  -32.147  41.974   8.040  1.00 50.12  A N
ATOM  212  CA  LEU A  62  -30.753  42.334   7.848  1.00 48.25  A C
ATOM  213  CB  LEU A  62  -29.950  42.074   9.123  1.00 48.23  A C
ATOM  214  CG  LEU A  62  -28.447  42.357   9.036  1.00 47.79  A C
ATOM  215  CD1 LEU A  62  -28.218  43.818   8.701  1.00 47.28  A C
ATOM  216  CD2 LEU A  62  -27.780  42.005  10.355  1.00 47.62  A C
ATOM  217  C   LEU A  62  -30.185  41.497   6.716  1.00 47.11  A C
ATOM  218  O   LEU A  62  -30.316  40.275   6.715  1.00 47.26  A O
ATOM  219  N   PRO A  63  -29.563  42.146   5.723  1.00 46.05  A N
ATOM  220  CD  PRO A  63  -29.397  43.598   5.535  1.00 45.82  A C
ATOM  221  CA  PRO A  63  -28.986  41.404   4.600  1.00 45.05  A C
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FIGURE 3A-5

```
ATOM  222  CB  PRO A  63   -28.646  42.505   3.599  1.00 45.21  A C
ATOM  223  CG  PRO A  63   -28.308  43.663   4.489  1.00 45.56  A C
ATOM  224  C   PRO A  63   -27.756  40.628   5.056  1.00 43.82  A C
ATOM  225  O   PRO A  63   -26.877  41.175   5.721  1.00 43.67  A O
ATOM  226  N   VAL A  64   -27.705  39.350   4.710  1.00 42.65  A N
ATOM  227  CA  VAL A  64   -26.578  38.517   5.097  1.00 41.36  A C
ATOM  228  CB  VAL A  64   -26.951  37.568   6.259  1.00 41.15  A C
ATOM  229  CG1 VAL A  64   -27.496  38.369   7.427  1.00 41.22  A C
ATOM  230  CG2 VAL A  64   -27.963  36.537   5.789  1.00 40.39  A C
ATOM  231  C   VAL A  64   -26.082  37.673   3.936  1.00 40.59  A C
ATOM  232  O   VAL A  64   -26.655  37.684   2.848  1.00 39.92  A O
ATOM  233  N   ALA A  65   -25.000  36.948   4.182  1.00 40.29  A N
ATOM  234  CA  ALA A  65   -24.418  36.067   3.187  1.00 39.95  A C
ATOM  235  CB  ALA A  65   -23.040  36.558   2.783  1.00 39.46  A C
ATOM  236  C   ALA A  65   -24.321  34.711   3.856  1.00 39.61  A C
ATOM  237  O   ALA A  65   -23.785  34.594   4.954  1.00 39.38  A O
ATOM  238  N   ILE A  66   -24.862  33.691   3.205  1.00 39.71  A N
ATOM  239  CA  ILE A  66   -24.824  32.350   3.762  1.00 39.78  A C
ATOM  240  CB  ILE A  66   -26.224  31.693   3.722  1.00 39.83  A C
ATOM  241  CG2 ILE A  66   -26.160  30.286   4.306  1.00 40.29  A C
ATOM  242  CG1 ILE A  66   -27.212  32.546   4.528  1.00 39.94  A C
ATOM  243  CD1 ILE A  66   -28.640  32.045   4.502  1.00 39.25  A C
ATOM  244  C   ILE A  66   -23.815  31.504   2.996  1.00 39.91  A C
ATOM  245  O   ILE A  66   -23.982  31.237   1.803  1.00 39.68  A O
ATOM  246  N   LYS A  67   -22.764  31.095   3.700  1.00 39.87  A N
ATOM  247  CA  LYS A  67   -21.694  30.297   3.122  1.00 40.15  A C
ATOM  248  CB  LYS A  67   -20.347  30.903   3.520  1.00 39.91  A C
ATOM  249  CG  LYS A  67   -19.137  30.359   2.786  1.00 39.52  A C
ATOM  250  CD  LYS A  67   -17.916  31.203   3.130  1.00 40.12  A C
ATOM  251  CE  LYS A  67   -16.695  30.813   2.313  1.00 40.55  A C
ATOM  252  NZ  LYS A  67   -15.587  31.793   2.497  1.00 40.25  A N
ATOM  253  C   LYS A  67   -21.771  28.844   3.578  1.00 40.52  A C
ATOM  254  O   LYS A  67   -21.816  28.554   4.772  1.00 40.27  A O
ATOM  255  N   HIS A  68   -21.793  27.936   2.611  1.00 41.40  A N
ATOM  256  CA  HIS A  68   -21.854  26.509   2.885  1.00 42.00  A C
ATOM  257  CB  HIS A  68   -22.940  25.855   2.032  1.00 41.61  A C
ATOM  258  CG  HIS A  68   -24.326  26.247   2.427  1.00 40.94  A C
ATOM  259  CD2 HIS A  68   -25.099  27.292   2.049  1.00 41.12  A C
ATOM  260  ND1 HIS A  68   -25.054  25.553   3.368  1.00 41.10  A N
ATOM  261  CE1 HIS A  68   -26.215  26.155   3.555  1.00 41.05  A C
ATOM  262  NE2 HIS A  68   -26.267  27.213   2.766  1.00 40.88  A N
ATOM  263  C   HIS A  68   -20.509  25.906   2.545  1.00 42.96  A C
ATOM  264  O   HIS A  68   -19.916  26.244   1.523  1.00 42.84  A O
ATOM  265  N   VAL A  69   -20.030  25.016   3.406  1.00 44.62  A N
ATOM  266  CA  VAL A  69   -18.746  24.367   3.192  1.00 46.68  A C
ATOM  267  CB  VAL A  69   -17.636  25.049   4.010  1.00 46.90  A C
ATOM  268  CG1 VAL A  69   -16.292  24.445   3.654  1.00 47.50  A C
ATOM  269  CG2 VAL A  69   -17.635  26.545   3.747  1.00 47.59  A C
ATOM  270  C   VAL A  69   -18.790  22.902   3.598  1.00 48.09  A C
ATOM  271  O   VAL A  69   -19.037  22.584   4.760  1.00 48.55  A O
ATOM  272  N   GLU A  70   -18.553  22.011   2.639  1.00 49.72  A N
ATOM  273  CA  GLU A  70   -18.546  20.581   2.924  1.00 51.13  A C

ATOM  274  CB  GLU A  70   -18.512  19.768   1.626  1.00 52.32  A C
ATOM  275  CG  GLU A  70   -19.840  19.713   0.888  1.00 54.34  A C
ATOM  276  CD  GLU A  70   -19.824  18.739  -0.276  1.00 55.69  A C
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FIGURE 3A-6

```
ATOM  277  OE1 GLU A  70   -19.531  17.543  -0.049  1.00 56.39   A O
ATOM  278  OE2 GLU A  70   -20.108  19.168  -1.418  1.00 56.29   A O
ATOM  279  C   GLU A  70   -17.314  20.260   3.758  1.00 51.41   A C
ATOM  280  O   GLU A  70   -16.226  20.767   3.482  1.00 51.30   A O
ATOM  281  N   LYS A  71   -17.489  19.423   4.778  1.00 51.81   A N
ATOM  282  CA  LYS A  71   -16.384  19.041   5.651  1.00 52.24   A C
ATOM  283  CB  LYS A  71   -16.891  18.180   6.804  1.00 51.33   A C
ATOM  284  CG  LYS A  71   -17.915  18.858   7.685  1.00 50.77   A C
ATOM  285  CD  LYS A  71   -18.343  17.928   8.804  1.00 50.35   A C
ATOM  286  CE  LYS A  71   -19.350  18.585   9.724  1.00 49.97   A C
ATOM  287  NZ  LYS A  71   -19.667  17.713  10.886  1.00 49.70   A N
ATOM  288  C   LYS A  71   -15.309  18.276   4.891  1.00 53.26   A C
ATOM  289  O   LYS A  71   -14.116  18.469   5.115  1.00 53.07   A O
ATOM  290  N   ASP A  72   -15.734  17.404   3.986  1.00 54.90   A N
ATOM  291  CA  ASP A  72   -14.789  16.617   3.210  1.00 56.76   A C
ATOM  292  CB  ASP A  72   -15.532  15.702   2.229  1.00 57.61   A C
ATOM  293  CG  ASP A  72   -16.353  14.626   2.931  1.00 58.94   A C
ATOM  294  OD1 ASP A  72   -17.087  13.888   2.235  1.00 59.46   A O
ATOM  295  OD2 ASP A  72   -16.266  14.511   4.175  1.00 59.32   A O
ATOM  296  C   ASP A  72   -13.820  17.503   2.442  1.00 57.46   A C
ATOM  297  O   ASP A  72   -12.742  17.059   2.065  1.00 58.11   A O
ATOM  298  N   ARG A  73   -14.192  18.760   2.227  1.00 58.37   A N
ATOM  299  CA  ARG A  73   -13.348  19.678   1.469  1.00 59.25   A C
ATOM  300  CB  ARG A  73   -14.216  20.489   0.505  1.00 59.89   A C
ATOM  301  CG  ARG A  73   -14.911  19.634  -0.536  1.00 61.24   A C
ATOM  302  CD  ARG A  73   -15.976  20.415  -1.284  1.00 62.70   A C
ATOM  303  NE  ARG A  73   -16.645  19.588  -2.285  1.00 63.75   A N
ATOM  304  CZ  ARG A  73   -17.674  19.993  -3.021  1.00 64.17   A C
ATOM  305  NH1 ARG A  73   -18.220  19.172  -3.910  1.00 64.29   A N
ATOM  306  NH2 ARG A  73   -18.162  21.216  -2.864  1.00 64.54   A N
ATOM  307  C   ARG A  73   -12.475  20.626   2.284  1.00 59.20   A C
ATOM  308  O   ARG A  73   -11.672  21.368   1.721  1.00 59.38   A O
ATOM  309  N   ILE A  74   -12.623  20.612   3.602  1.00 59.21   A N
ATOM  310  CA  ILE A  74   -11.820  21.491   4.440  1.00 59.33   A C
ATOM  311  CB  ILE A  74   -12.445  21.647   5.838  1.00 58.82   A C
ATOM  312  CG2 ILE A  74   -11.558  22.522   6.710  1.00 58.40   A C
ATOM  313  CG1 ILE A  74   -13.847  22.250   5.707  1.00 58.36   A C
ATOM  314  CD1 ILE A  74   -14.586  22.406   7.019  1.00 57.92   A C
ATOM  315  C   ILE A  74   -10.411  20.926   4.573  1.00 59.93   A C
ATOM  316  O   ILE A  74   -10.237  19.717   4.722  1.00 60.16   A O
ATOM  317  N   SER A  75    -9.410  21.803   4.516  1.00 60.45   A N
ATOM  318  CA  SER A  75    -8.013  21.384   4.622  1.00 60.66   A C
ATOM  319  CB  SER A  75    -7.203  21.995   3.480  1.00 60.78   A C
ATOM  320  OG  SER A  75    -7.753  21.628   2.226  1.00 60.84   A O
ATOM  321  C   SER A  75    -7.382  21.758   5.965  1.00 60.90   A C
ATOM  322  O   SER A  75    -6.552  21.014   6.494  1.00 60.88   A O
ATOM  323  N   ASP A  76    -7.775  22.911   6.506  1.00 60.99   A N
ATOM  324  CA  ASP A  76    -7.263  23.384   7.791  1.00 60.77   A C
ATOM  325  CB  ASP A  76    -6.572  24.738   7.640  1.00 61.29   A C
ATOM  326  CG  ASP A  76    -5.247  24.638   6.933  1.00 62.10   A C
ATOM  327  OD1 ASP A  76    -4.523  25.657   6.890  1.00 62.78   A O
ATOM  328  OD2 ASP A  76    -4.931  23.544   6.418  1.00 62.85   A O
ATOM  329  C   ASP A  76    -8.379  23.534   8.811  1.00 60.45   A C
ATOM  330  O   ASP A  76    -9.368  24.217   8.557  1.00 60.57   A O
ATOM  331  N   TRP A  77    -8.211  22.907   9.970  1.00 59.95   A N
ATOM  332  CA  TRP A  77    -9.208  22.991  11.028  1.00 59.65   A C
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FIGURE 3A-7

```
ATOM  333  CB  TRP A  77    -9.661  21.591  11.453  1.00 59.18  A C
ATOM  334  CG  TRP A  77   -10.294  20.772  10.366  1.00 58.20  A C
ATOM  335  CD2 TRP A  77   -11.670  20.386  10.279  1.00 57.75  A C
ATOM  336  CE2 TRP A  77   -11.811  19.600   9.115  1.00 57.52  A C
ATOM  337  CE3 TRP A  77   -12.798  20.625  11.075  1.00 57.64  A C
ATOM  338  CD1 TRP A  77    -9.673  20.226   9.280  1.00 57.99  A C
ATOM  339  NE1 TRP A  77   -10.578  19.518   8.523  1.00 57.72  A N
ATOM  340  CZ2 TRP A  77   -13.036  19.053   8.724  1.00 57.29  A C
ATOM  341  CZ3 TRP A  77   -14.020  20.080  10.685  1.00 57.58  A C
ATOM  342  CH2 TRP A  77   -14.126  19.301   9.520  1.00 57.19  A C
ATOM  343  C   TRP A  77    -8.635  23.721  12.240  1.00 59.84  A C
ATOM  344  O   TRP A  77    -7.449  23.601  12.541  1.00 59.94  A O
ATOM  345  N   GLY A  78    -9.482  24.473  12.934  1.00 59.96  A N
ATOM  346  CA  GLY A  78    -9.032  25.203  14.107  1.00 60.19  A C
ATOM  347  C   GLY A  78    -9.793  24.779  15.347  1.00 60.30  A C
ATOM  348  O   GLY A  78   -10.607  23.859  15.286  1.00 60.64  A O
ATOM  349  N   ALA A  79    -9.536  25.444  16.470  1.00 60.12  A N
ATOM  350  CA  ALA A  79   -10.211  25.117  17.721  1.00 60.23  A C
ATOM  351  CB  ALA A  79    -9.193  24.992  18.847  1.00 60.37  A C
ATOM  352  C   ALA A  79   -11.261  26.162  18.082  1.00 60.36  A C
ATOM  353  O   ALA A  79   -11.520  26.419  19.261  1.00 60.53  A O
ATOM  354  N   THR A  84   -13.418  21.930  20.215  1.00 56.12  A N
ATOM  355  CA  THR A  84   -14.190  21.600  19.021  1.00 56.31  A C
ATOM  356  CB  THR A  84   -15.644  22.088  19.147  1.00 56.55  A C
ATOM  357  OG1 THR A  84   -15.673  23.312  19.892  1.00 55.88  A O
ATOM  358  CG2 THR A  84   -16.502  21.032  19.840  1.00 56.81  A C
ATOM  359  C   THR A  84   -13.588  22.185  17.747  1.00 56.34  A C
ATOM  360  O   THR A  84   -13.376  23.395  17.637  1.00 56.44  A O
ATOM  361  N   ARG A  85   -13.325  21.308  16.784  1.00 56.07  A N
ATOM  362  CA  ARG A  85   -12.738  21.704  15.512  1.00 55.70  A C
ATOM  363  CB  ARG A  85   -12.186  20.472  14.797  1.00 56.26  A C
ATOM  364  CG  ARG A  85   -11.210  19.659  15.630  1.00 57.07  A C
ATOM  365  CD  ARG A  85   -10.989  18.297  15.000  1.00 57.98  A C
ATOM  366  NE  ARG A  85   -10.311  18.388  13.711  1.00 58.76  A N
ATOM  367  CZ  ARG A  85   -10.507  17.545  12.702  1.00 59.06  A C
ATOM  368  NH1 ARG A  85   -11.371  16.544  12.827  1.00 59.18  A N
ATOM  369  NH2 ARG A  85    -9.833  17.697  11.569  1.00 59.13  A N
ATOM  370  C   ARG A  85   -13.758  22.399  14.617  1.00 55.04  A C
ATOM  371  O   ARG A  85   -14.948  22.096  14.667  1.00 55.19  A O
ATOM  372  N   VAL A  86   -13.277  23.329  13.797  1.00 53.87  A N
ATOM  373  CA  VAL A  86   -14.125  24.085  12.878  1.00 52.21  A C
ATOM  374  CB  VAL A  86   -14.766  25.308  13.586  1.00 51.90  A C
ATOM  375  CG1 VAL A  86   -15.730  24.849  14.666  1.00 51.57  A C
ATOM  376  CG2 VAL A  86   -13.683  26.181  14.197  1.00 51.51  A C
ATOM  377  C   VAL A  86   -13.252  24.591  11.729  1.00 51.29  A C
ATOM  378  O   VAL A  86   -12.025  24.528  11.804  1.00 51.44  A O
ATOM  379  N   PRO A  87   -13.869  25.086  10.643  1.00 50.30  A N
ATOM  380  CD  PRO A  87   -15.305  25.156  10.320  1.00 50.21  A C
ATOM  381  CA  PRO A  87   -13.059  25.587   9.527  1.00 49.25  A C
ATOM  382  CB  PRO A  87   -14.095  25.828   8.429  1.00 49.33  A C
ATOM  383  CG  PRO A  87   -15.328  26.170   9.198  1.00 49.66  A C
ATOM  384  C   PRO A  87   -12.294  26.861   9.907  1.00 48.26  A C
ATOM  385  O   PRO A  87   -12.817  27.722  10.619  1.00 48.06  A O
ATOM  386  N   MET A  88   -11.055  26.967   9.436  1.00 47.05  A N
ATOM  387  CA  MET A  88   -10.215  28.124   9.720  1.00 46.01  A C
ATOM  388  CB  MET A  88    -9.086  28.219   8.694  1.00 46.46  A C
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FIGURE 3A-8

```
ATOM  389  CG  MET A  88    -7.735  27.773   9.217  1.00 46.81  A C
ATOM  390  SD  MET A  88    -7.268  28.645  10.725  1.00 47.64  A S
ATOM  391  CE  MET A  88    -7.116  27.279  11.871  1.00 47.45  A C
ATOM  392  C   MET A  88   -10.982  29.440   9.731  1.00 45.15  A C
ATOM  393  O   MET A  88   -10.862  30.232  10.665  1.00 45.06  A O
ATOM  394  N   GLU A  89   -11.765  29.665   8.683  1.00 43.92  A N
ATOM  395  CA  GLU A  89   -12.552  30.885   8.545  1.00 42.97  A C
ATOM  396  CB  GLU A  89   -13.647  30.688   7.498  1.00 44.25  A C
ATOM  397  CG  GLU A  89   -13.166  30.156   6.161  1.00 45.95  A C
ATOM  398  CD  GLU A  89   -14.318  29.779   5.242  1.00 46.96  A C
ATOM  399  OE1 GLU A  89   -15.160  30.661   4.948  1.00 46.95  A O
ATOM  400  OE2 GLU A  89   -14.379  28.602   4.818  1.00 46.92  A O
ATOM  401  C   GLU A  89   -13.208  31.325   9.846  1.00 41.46  A C
ATOM  402  O   GLU A  89   -13.160  32.502  10.201  1.00 41.15  A O
ATOM  403  N   VAL A  90   -13.825  30.374  10.543  1.00 40.04  A N
ATOM  404  CA  VAL A  90   -14.524  30.654  11.795  1.00 38.60  A C
ATOM  405  CB  VAL A  90   -15.300  29.419  12.299  1.00 38.25  A C
ATOM  406  CG1 VAL A  90   -16.072  29.774  13.557  1.00 37.96  A C
ATOM  407  CG2 VAL A  90   -16.243  28.919  11.222  1.00 38.04  A C
ATOM  408  C   VAL A  90   -13.595  31.115  12.907  1.00 37.86  A C
ATOM  409  O   VAL A  90   -13.903  32.070  13.614  1.00 37.85  A O
ATOM  410  N   VAL A  91   -12.468  30.432  13.071  1.00 37.25  A N
ATOM  411  CA  VAL A  91   -11.512  30.805  14.107  1.00 36.71  A C
ATOM  412  CB  VAL A  91   -10.357  29.790  14.192  1.00 36.51  A C
ATOM  413  CG1 VAL A  91    -9.332  30.254  15.205  1.00 36.25  A C
ATOM  414  CG2 VAL A  91   -10.898  28.427  14.586  1.00 36.46  A C
ATOM  415  C   VAL A  91   -10.940  32.191  13.816  1.00 36.51  A C
ATOM  416  O   VAL A  91   -10.971  33.084  14.666  1.00 36.34  A O
ATOM  417  N   LEU A  92   -10.434  32.367  12.602  1.00 35.95  A N
ATOM  418  CA  LEU A  92    -9.852  33.633  12.188  1.00 35.63  A C
ATOM  419  CB  LEU A  92    -9.350  33.517  10.746  1.00 35.03  A C
ATOM  420  CG  LEU A  92    -8.336  32.385  10.524  1.00 34.80  A C
ATOM  421  CD1 LEU A  92    -8.000  32.274   9.048  1.00 34.36  A C
ATOM  422  CD2 LEU A  92    -7.078  32.641  11.348  1.00 33.97  A C
ATOM  423  C   LEU A  92   -10.830  34.799  12.321  1.00 35.89  A C
ATOM  424  O   LEU A  92   -10.516  35.805  12.956  1.00 35.88  A O
ATOM  425  N   LEU A  93   -12.015  34.666  11.735  1.00 36.47  A N
ATOM  426  CA  LEU A  93   -13.012  35.731  11.807  1.00 37.19  A C
ATOM  427  CB  LEU A  93   -14.252  35.360  10.990  1.00 37.08  A C
ATOM  428  CG  LEU A  93   -14.096  35.470   9.472  1.00 37.32  A C
ATOM  429  CD1 LEU A  93   -15.350  34.963   8.786  1.00 37.12  A C
ATOM  430  CD2 LEU A  93   -13.820  36.918   9.089  1.00 36.90  A C
ATOM  431  C   LEU A  93   -13.417  36.071  13.239  1.00 37.96  A C
ATOM  432  O   LEU A  93   -13.746  37.217  13.539  1.00 38.01  A O
ATOM  433  N   LYS A  94   -13.395  35.082  14.123  1.00 39.01  A N
ATOM  434  CA  LYS A  94   -13.753  35.324  15.516  1.00 40.43  A C
ATOM  435  CB  LYS A  94   -13.920  34.005  16.274  1.00 40.84  A C
ATOM  436  CG  LYS A  94   -15.295  33.375  16.154  1.00 41.21  A C
ATOM  437  CD  LYS A  94   -15.388  32.130  17.022  1.00 42.02  A C
ATOM  438  CE  LYS A  94   -16.824  31.638  17.142  1.00 43.55  A C
ATOM  439  NZ  LYS A  94   -17.723  32.632  17.812  1.00 43.93  A N
ATOM  440  C   LYS A  94   -12.690  36.165  16.210  1.00 41.26  A C
ATOM  441  O   LYS A  94   -12.991  36.903  17.147  1.00 41.25  A O
ATOM  442  N   LYS A  95   -11.447  36.046  15.748  1.00 42.23  A N
ATOM  443  CA  LYS A  95   -10.344  36.799  16.335  1.00 43.35  A C
ATOM  444  CB  LYS A  95    -9.007  36.148  15.975  1.00 42.39  A C
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FIGURE 3A-9

```
ATOM   445  CG  LYS A  95     -8.867  34.713  16.452  1.00 41.88   A C
ATOM   446  CD  LYS A  95     -7.425  34.236  16.359  1.00 41.24   A C
ATOM   447  CE  LYS A  95     -6.542  34.991  17.335  1.00 40.96   A C
ATOM   448  NZ  LYS A  95     -5.136  34.528  17.269  1.00 41.24   A N
ATOM   449  C   LYS A  95    -10.333  38.264  15.897  1.00 44.57   A C
ATOM   450  O   LYS A  95     -9.951  39.148  16.667  1.00 44.22   A O
ATOM   451  N   VAL A  96    -10.755  38.520  14.663  1.00 46.07   A N
ATOM   452  CA  VAL A  96    -10.782  39.878  14.144  1.00 48.00   A C
ATOM   453  CB  VAL A  96    -10.461  39.898  12.638  1.00 47.72   A C
ATOM   454  CG1 VAL A  96     -9.016  39.502  12.421  1.00 47.78   A C
ATOM   455  CG2 VAL A  96    -11.372  38.940  11.891  1.00 47.72   A C
ATOM   456  C   VAL A  96    -12.124  40.556  14.382  1.00 49.75   A C
ATOM   457  O   VAL A  96    -12.224  41.468  15.206  1.00 49.82   A O
ATOM   458  N   SER A  97    -13.145  40.094  13.661  1.00 51.89   A N
ATOM   459  CA  SER A  97    -14.511  40.623  13.745  1.00 53.86   A C
ATOM   460  CB  SER A  97    -15.521  39.477  13.913  1.00 53.93   A C
ATOM   461  OG  SER A  97    -15.629  38.698  12.734  1.00 54.06   A O
ATOM   462  C   SER A  97    -14.741  41.640  14.855  1.00 54.86   A C
ATOM   463  O   SER A  97    -14.812  42.843  14.598  1.00 54.69   A O
ATOM   464  N   SER A  98    -14.864  41.141  16.084  1.00 56.00   A N
ATOM   465  CA  SER A  98    -15.101  41.984  17.250  1.00 56.78   A C
ATOM   466  CB  SER A  98    -14.348  41.433  18.463  1.00 57.23   A C
ATOM   467  OG  SER A  98    -14.694  42.142  19.645  1.00 58.13   A O
ATOM   468  C   SER A  98    -14.687  43.427  16.993  1.00 56.97   A C
ATOM   469  O   SER A  98    -13.510  43.721  16.758  1.00 56.70   A O
ATOM   470  N   GLY A  99    -15.674  44.316  17.018  1.00 57.31   A N
ATOM   471  CA  GLY A  99    -15.416  45.722  16.787  1.00 57.20   A C
ATOM   472  C   GLY A  99    -15.605  46.116  15.338  1.00 57.02   A C
ATOM   473  O   GLY A  99    -15.755  45.268  14.457  1.00 56.92   A O
ATOM   474  N   PHE A 100    -15.602  47.419  15.091  1.00 56.74   A N
ATOM   475  CA  PHE A 100    -15.755  47.949  13.746  1.00 56.15   A C
ATOM   476  CB  PHE A 100    -16.039  49.457  13.823  1.00 57.23   A C
ATOM   477  CG  PHE A 100    -17.382  49.807  14.427  1.00 58.27   A C
ATOM   478  CD1 PHE A 100    -17.590  51.062  15.014  1.00 58.56   A C
ATOM   479  CD2 PHE A 100    -18.448  48.911  14.372  1.00 58.73   A C
ATOM   480  CE1 PHE A 100    -18.848  51.413  15.536  1.00 59.14   A C
ATOM   481  CE2 PHE A 100    -19.707  49.250  14.889  1.00 58.98   A C
ATOM   482  CZ  PHE A 100    -19.907  50.501  15.470  1.00 59.30   A C
ATOM   483  C   PHE A 100    -14.471  47.692  12.966  1.00 55.26   A C
ATOM   484  O   PHE A 100    -13.401  47.566  13.562  1.00 55.13   A O
ATOM   485  N   SER A 101    -14.576  47.609  11.642  1.00 53.94   A N
ATOM   486  CA  SER A 101    -13.393  47.385  10.819  1.00 52.77   A C
ATOM   487  CB  SER A 101    -12.568  46.211  11.367  1.00 53.28   A C
ATOM   488  OG  SER A 101    -11.236  46.281  10.911  1.00 53.94   A O
ATOM   489  C   SER A 101    -13.714  47.136   9.346  1.00 51.37   A C
ATOM   490  O   SER A 101    -14.879  47.118   8.933  1.00 51.14   A O
ATOM   491  N   GLY A 102    -12.661  46.942   8.557  1.00 49.52   A N
ATOM   492  CA  GLY A 102    -12.819  46.694   7.134  1.00 46.92   A C
ATOM   493  C   GLY A 102    -12.755  45.218   6.788  1.00 45.27   A C
ATOM   494  O   GLY A 102    -12.297  44.851   5.707  1.00 44.33   A O
ATOM   495  N   VAL A 103    -13.197  44.372   7.712  1.00 44.29   A N
ATOM   496  CA  VAL A 103    -13.220  42.940   7.472  1.00 43.70   A C
ATOM   497  CB  VAL A 103    -12.305  42.153   8.465  1.00 43.74   A C
ATOM   498  CG1 VAL A 103    -10.873  42.643   8.368  1.00 43.81   A C
ATOM   499  CG2 VAL A 103    -12.812  42.289   9.884  1.00 44.07   A C
ATOM   500  C   VAL A 103    -14.658  42.450   7.629  1.00 43.05   A C
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FIGURE 3A-10

```
ATOM   501  O   VAL A 103   -15.349   42.834    8.574  1.00 42.67   A O
ATOM   502  N   ILE A 104   -15.118   41.622    6.696  1.00 42.53   A N
ATOM   503  CA  ILE A 104   -16.469   41.083    6.780  1.00 42.38   A C
ATOM   504  CB  ILE A 104   -16.747   40.051    5.655  1.00 42.24   A C
ATOM   505  CG2 ILE A 104   -17.739   38.996    6.125  1.00 42.60   A C
ATOM   506  CG1 ILE A 104   -17.295   40.765    4.420  1.00 42.46   A C
ATOM   507  CD1 ILE A 104   -18.660   41.383    4.606  1.00 41.93   A C
ATOM   508  C   ILE A 104   -16.629   40.413    8.137  1.00 42.45   A C
ATOM   509  O   ILE A 104   -15.749   39.679    8.584  1.00 42.84   A O
ATOM   510  N   ARG A 105   -17.752   40.669    8.794  1.00 42.44   A N
ATOM   511  CA  ARG A 105   -17.990   40.094   10.109  1.00 42.79   A C
ATOM   512  CB  ARG A 105   -18.727   41.107   10.988  1.00 44.78   A C
ATOM   513  CG  ARG A 105   -18.038   42.462   11.018  1.00 48.43   A C
ATOM   514  CD  ARG A 105   -18.544   43.360   12.136  1.00 51.14   A C
ATOM   515  NE  ARG A 105   -18.160   42.858   13.453  1.00 53.54   A N
ATOM   516  CZ  ARG A 105   -18.054   43.619   14.538  1.00 54.70   A C
ATOM   517  NH1 ARG A 105   -18.303   44.922   14.464  1.00 55.14   A N
ATOM   518  NH2 ARG A 105   -17.692   43.079   15.697  1.00 55.31   A N
ATOM   519  C   ARG A 105   -18.752   38.773   10.094  1.00 41.55   A C
ATOM   520  O   ARG A 105   -19.628   38.551    9.257  1.00 41.18   A O
ATOM   521  N   LEU A 106   -18.394   37.893   11.023  1.00 40.34   A N
ATOM   522  CA  LEU A 106   -19.053   36.603   11.151  1.00 39.37   A C
ATOM   523  CB  LEU A 106   -18.085   35.551   11.691  1.00 38.49   A C
ATOM   524  CG  LEU A 106   -18.699   34.157   11.820  1.00 37.96   A C
ATOM   525  CD1 LEU A 106   -19.006   33.616   10.431  1.00 37.17   A C
ATOM   526  CD2 LEU A 106   -17.745   33.234   12.565  1.00 37.69   A C
ATOM   527  C   LEU A 106   -20.201   36.787   12.133  1.00 39.12   A C
ATOM   528  O   LEU A 106   -19.987   36.935   13.335  1.00 38.80   A O
ATOM   529  N   LEU A 107   -21.420   36.789   11.614  1.00 39.02   A N
ATOM   530  CA  LEU A 107   -22.595   36.969   12.448  1.00 39.65   A C
ATOM   531  CB  LEU A 107   -23.795   37.335   11.570  1.00 39.17   A C
ATOM   532  CG  LEU A 107   -24.063   38.828   11.346  1.00 38.64   A C
ATOM   533  CD1 LEU A 107   -22.775   39.626   11.420  1.00 38.46   A C
ATOM   534  CD2 LEU A 107   -24.754   39.018   10.003  1.00 38.77   A C
ATOM   535  C   LEU A 107   -22.901   35.734   13.283  1.00 40.22   A C
ATOM   536  O   LEU A 107   -23.268   35.843   14.451  1.00 39.68   A O
ATOM   537  N   ASP A 108   -22.740   34.561   12.682  1.00 41.33   A N
ATOM   538  CA  ASP A 108   -23.006   33.309   13.373  1.00 42.49   A C
ATOM   539  CB  ASP A 108   -24.481   33.261   13.795  1.00 43.83   A C
ATOM   540  CG  ASP A 108   -24.850   31.978   14.522  1.00 45.09   A C
ATOM   541  OD1 ASP A 108   -23.976   31.390   15.196  1.00 45.99   A O
ATOM   542  OD2 ASP A 108   -26.028   31.569   14.431  1.00 45.66   A O
ATOM   543  C   ASP A 108   -22.667   32.143   12.454  1.00 42.56   A C
ATOM   544  O   ASP A 108   -22.482   32.326   11.255  1.00 42.66   A O
ATOM   545  N   TRP A 109   -22.570   30.946   13.018  1.00 43.16   A N
ATOM   546  CA  TRP A 109   -22.256   29.768   12.222  1.00 43.88   A C
ATOM   547  CB  TRP A 109   -20.742   29.544   12.176  1.00 43.70   A C
ATOM   548  CG  TRP A 109   -20.130   29.290   13.519  1.00 43.65   A C
ATOM   549  CD2 TRP A 109   -19.816   28.014   14.089  1.00 43.65   A C
ATOM   550  CE2 TRP A 109   -19.287   28.250   15.375  1.00 43.35   A C
ATOM   551  CE3 TRP A 109   -19.934   26.692   13.636  1.00 43.61   A C
ATOM   552  CD1 TRP A 109   -19.788   30.221   14.455  1.00 43.48   A C
ATOM   553  NE1 TRP A 109   -19.280   29.605   15.573  1.00 43.49   A N
ATOM   554  CZ2 TRP A 109   -18.874   27.213   16.217  1.00 43.56   A C
ATOM   555  CZ3 TRP A 109   -19.522   25.657   14.476  1.00 43.63   A C
ATOM   556  CH2 TRP A 109   -19.000   25.926   15.752  1.00 43.51   A C
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FIGURE 3A-11

```
ATOM  557  C   TRP A 109  -22.943  28.527  12.785  1.00 44.28  A C
ATOM  558  O   TRP A 109  -23.217  28.452  13.985  1.00 44.47  A O
ATOM  559  N   PHE A 110  -23.224  27.562  11.910  1.00 44.49  A N
ATOM  560  CA  PHE A 110  -23.875  26.312  12.302  1.00 44.40  A C
ATOM  561  CB  PHE A 110  -25.316  26.243  11.784  1.00 45.03  A C
ATOM  562  CG  PHE A 110  -26.162  27.424  12.152  1.00 45.88  A C
ATOM  563  CD1 PHE A 110  -26.200  28.548  11.338  1.00 46.28  A C
ATOM  564  CD2 PHE A 110  -26.937  27.406  13.306  1.00 46.50  A C
ATOM  565  CE1 PHE A 110  -27.001  29.641  11.668  1.00 47.01  A C
ATOM  566  CE2 PHE A 110  -27.742  28.491  13.647  1.00 46.95  A C
ATOM  567  CZ  PHE A 110  -27.774  29.611  12.825  1.00 47.12  A C
ATOM  568  C   PHE A 110  -23.128  25.120  11.729  1.00 44.07  A C
ATOM  569  O   PHE A 110  -22.594  25.184  10.623  1.00 43.90  A O
ATOM  570  N   GLU A 111  -23.093  24.028  12.482  1.00 44.03  A N
ATOM  571  CA  GLU A 111  -22.438  22.819  12.006  1.00 44.13  A C
ATOM  572  CB  GLU A 111  -21.529  22.212  13.077  1.00 43.99  A C
ATOM  573  CG  GLU A 111  -21.121  20.778  12.765  1.00 43.47  A C
ATOM  574  CD  GLU A 111  -20.092  20.235  13.729  1.00 43.95  A C
ATOM  575  OE1 GLU A 111  -20.175  20.555  14.932  1.00 44.50  A O
ATOM  576  OE2 GLU A 111  -19.204  19.477  13.288  1.00 43.93  A O
ATOM  577  C   GLU A 111  -23.504  21.810  11.626  1.00 44.13  A C
ATOM  578  O   GLU A 111  -24.494  21.640  12.339  1.00 43.98  A O
ATOM  579  N   ARG A 112  -23.305  21.148  10.494  1.00 43.98  A N
ATOM  580  CA  ARG A 112  -24.252  20.153  10.033  1.00 43.95  A C
ATOM  581  CB  ARG A 112  -24.966  20.655   8.774  1.00 43.12  A C
ATOM  582  CG  ARG A 112  -25.557  22.033   9.002  1.00 42.57  A C
ATOM  583  CD  ARG A 112  -26.901  22.249   8.349  1.00 42.02  A C
ATOM  584  NE  ARG A 112  -26.803  22.457   6.911  1.00 41.93  A N
ATOM  585  CZ  ARG A 112  -27.768  23.002   6.178  1.00 41.48  A C
ATOM  586  NH1 ARG A 112  -28.897  23.396   6.752  1.00 41.24  A N
ATOM  587  NH2 ARG A 112  -27.608  23.153   4.872  1.00 41.49  A N
ATOM  588  C   ARG A 112  -23.491  18.863   9.779  1.00 44.48  A C
ATOM  589  O   ARG A 112  -22.271  18.874   9.620  1.00 44.46  A O
ATOM  590  N   PRO A 113  -24.202  17.729   9.760  1.00 44.90  A N
ATOM  591  CD  PRO A 113  -25.670  17.584   9.840  1.00 44.98  A C
ATOM  592  CA  PRO A 113  -23.562  16.434   9.532  1.00 44.95  A C
ATOM  593  CB  PRO A 113  -24.724  15.570   9.053  1.00 45.01  A C
ATOM  594  CG  PRO A 113  -25.854  16.076   9.912  1.00 45.06  A C
ATOM  595  C   PRO A 113  -22.381  16.440   8.563  1.00 44.84  A C
ATOM  596  O   PRO A 113  -21.299  15.970   8.906  1.00 44.74  A O
ATOM  597  N   ASP A 114  -22.576  16.989   7.367  1.00 45.06  A N
ATOM  598  CA  ASP A 114  -21.512  17.007   6.366  1.00 45.07  A C
ATOM  599  CB  ASP A 114  -21.964  16.226   5.139  1.00 46.61  A C
ATOM  600  CG  ASP A 114  -22.267  14.779   5.459  1.00 48.43  A C
ATOM  601  OD1 ASP A 114  -21.311  14.026   5.757  1.00 49.40  A O
ATOM  602  OD2 ASP A 114  -23.460  14.398   5.421  1.00 48.88  A O
ATOM  603  C   ASP A 114  -21.017  18.379   5.925  1.00 44.16  A C
ATOM  604  O   ASP A 114  -20.358  18.498   4.893  1.00 44.44  A O
ATOM  605  N   SER A 115  -21.316  19.413   6.698  1.00 42.81  A N
ATOM  606  CA  SER A 115  -20.875  20.747   6.323  1.00 41.24  A C
ATOM  607  CB  SER A 115  -21.594  21.197   5.044  1.00 41.03  A C
ATOM  608  OG  SER A 115  -22.998  21.260   5.232  1.00 40.14  A O
ATOM  609  C   SER A 115  -21.109  21.775   7.413  1.00 40.29  A C
ATOM  610  O   SER A 115  -21.759  21.500   8.425  1.00 39.77  A O
ATOM  611  N   PHE A 116  -20.556  22.963   7.193  1.00 39.27  A N
ATOM  612  CA  PHE A 116  -20.707  24.080   8.114  1.00 38.15  A C
```

FIGURE 3A-12

```
ATOM  613  CB  PHE A 116  -19.347  24.590   8.595  1.00 37.80  A C
ATOM  614  CG  PHE A 116  -18.681  23.700   9.597  1.00 37.37  A C
ATOM  615  CD1 PHE A 116  -17.838  22.672   9.186  1.00 37.07  A C
ATOM  616  CD2 PHE A 116  -18.896  23.891  10.957  1.00 37.13  A C
ATOM  617  CE1 PHE A 116  -17.217  21.849  10.117  1.00 36.45  A C
ATOM  618  CE2 PHE A 116  -18.282  23.075  11.895  1.00 36.55  A C
ATOM  619  CZ  PHE A 116  -17.440  22.052  11.474  1.00 36.83  A C
ATOM  620  C   PHE A 116  -21.402  25.197   7.367  1.00 37.04  A C
ATOM  621  O   PHE A 116  -21.240  25.333   6.160  1.00 37.55  A O
ATOM  622  N   VAL A 117  -22.181  25.994   8.079  1.00 36.15  A N
ATOM  623  CA  VAL A 117  -22.866  27.112   7.454  1.00 35.45  A C
ATOM  624  CB  VAL A 117  -24.395  26.964   7.529  1.00 35.21  A C
ATOM  625  CG1 VAL A 117  -25.062  28.159   6.866  1.00 34.90  A C
ATOM  626  CG2 VAL A 117  -24.820  25.680   6.848  1.00 35.28  A C
ATOM  627  C   VAL A 117  -22.456  28.373   8.188  1.00 35.20  A C
ATOM  628  O   VAL A 117  -22.632  28.479   9.404  1.00 35.12  A O
ATOM  629  N   LEU A 118  -21.889  29.321   7.450  1.00 34.96  A N
ATOM  630  CA  LEU A 118  -21.455  30.579   8.041  1.00 34.30  A C
ATOM  631  CB  LEU A 118  -20.020  30.914   7.617  1.00 34.25  A C
ATOM  632  CG  LEU A 118  -18.882  30.130   8.271  1.00 34.28  A C
ATOM  633  CD1 LEU A 118  -18.986  28.665   7.908  1.00 33.92  A C
ATOM  634  CD2 LEU A 118  -17.552  30.692   7.809  1.00 34.48  A C
ATOM  635  C   LEU A 118  -22.370  31.718   7.641  1.00 33.76  A C
ATOM  636  O   LEU A 118  -22.738  31.857   6.476  1.00 33.44  A O
ATOM  637  N   ILE A 119  -22.745  32.527   8.620  1.00 33.37  A N
ATOM  638  CA  ILE A 119  -23.591  33.672   8.361  1.00 33.43  A C
ATOM  639  CB  ILE A 119  -24.692  33.816   9.438  1.00 33.56  A C
ATOM  640  CG2 ILE A 119  -25.592  34.999   9.108  1.00 33.63  A C
ATOM  641  CG1 ILE A 119  -25.522  32.535   9.509  1.00 32.95  A C
ATOM  642  CD1 ILE A 119  -26.188  32.161   8.202  1.00 32.94  A C
ATOM  643  C   ILE A 119  -22.688  34.897   8.390  1.00 33.60  A C
ATOM  644  O   ILE A 119  -22.243  35.329   9.455  1.00 33.82  A O
ATOM  645  N   LEU A 120  -22.393  35.434   7.210  1.00 33.68  A N
ATOM  646  CA  LEU A 120  -21.545  36.613   7.090  1.00 33.81  A C
ATOM  647  CB  LEU A 120  -20.534  36.449   5.951  1.00 32.42  A C
ATOM  648  CG  LEU A 120  -19.390  35.436   6.032  1.00 31.75  A C
ATOM  649  CD1 LEU A 120  -18.801  35.474   7.430  1.00 31.38  A C
ATOM  650  CD2 LEU A 120  -19.875  34.047   5.693  1.00 31.01  A C
ATOM  651  C   LEU A 120  -22.411  37.825   6.792  1.00 34.85  A C
ATOM  652  O   LEU A 120  -23.500  37.694   6.240  1.00 35.02  A O
ATOM  653  N   GLU A 121  -21.928  39.008   7.150  1.00 36.10  A N
ATOM  654  CA  GLU A 121  -22.687  40.216   6.878  1.00 37.40  A C
ATOM  655  CB  GLU A 121  -22.061  41.422   7.580  1.00 37.97  A C
ATOM  656  CG  GLU A 121  -20.900  42.055   6.823  1.00 38.66  A C
ATOM  657  CD  GLU A 121  -20.249  43.197   7.584  1.00 39.42  A C
ATOM  658  OE1 GLU A 121  -19.770  42.950   8.711  1.00 40.01  A O
ATOM  659  OE2 GLU A 121  -20.215  44.335   7.060  1.00 39.26  A O
ATOM  660  C   GLU A 121  -22.659  40.435   5.371  1.00 37.96  A C
ATOM  661  O   GLU A 121  -21.763  39.943   4.682  1.00 37.98  A O
ATOM  662  N   ARG A 122  -23.646  41.159   4.857  1.00 38.94  A N
ATOM  663  CA  ARG A 122  -23.708  41.456   3.430  1.00 39.63  A C
ATOM  664  CB  ARG A 122  -24.655  40.505   2.694  1.00 39.47  A C
ATOM  665  CG  ARG A 122  -24.886  40.905   1.233  1.00 39.76  A C
ATOM  666  CD  ARG A 122  -25.607  39.827   0.428  1.00 39.91  A C
ATOM  667  NE  ARG A 122  -26.966  39.573   0.900  1.00 40.40  A N
ATOM  668  CZ  ARG A 122  -27.999  40.386   0.700  1.00 40.64  A C
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FIGURE 3A-13

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ATOM  669  NH1 ARG A 122  -27.844  41.518   0.029  1.00 40.48  A N
ATOM  670  NH2 ARG A 122  -29.191  40.070   1.182  1.00 40.87  A N
ATOM  671  C   ARG A 122  -24.172  42.884   3.212  1.00 40.02  A C
ATOM  672  O   ARG A 122  -25.291  43.245   3.571  1.00 40.16  A O
ATOM  673  N   PRO A 123  -23.296  43.730   2.653  1.00 40.37  A N
ATOM  674  CD  PRO A 123  -21.826  43.588   2.625  1.00 40.29  A C
ATOM  675  CA  PRO A 123  -23.690  45.120   2.411  1.00 40.78  A C
ATOM  676  CB  PRO A 123  -22.374  45.877   2.572  1.00 40.77  A C
ATOM  677  CG  PRO A 123  -21.374  44.911   2.041  1.00 40.05  A C
ATOM  678  C   PRO A 123  -24.307  45.288   1.024  1.00 41.14  A C
ATOM  679  O   PRO A 123  -23.849  44.689   0.057  1.00 41.69  A O
ATOM  680  N   GLU A 124  -25.366  46.083   0.951  1.00 41.64  A N
ATOM  681  CA  GLU A 124  -26.077  46.356  -0.292  1.00 42.34  A C
ATOM  682  CB  GLU A 124  -27.418  45.600  -0.311  1.00 43.95  A C
ATOM  683  CG  GLU A 124  -28.641  46.389  -0.837  1.00 46.92  A C
ATOM  684  CD  GLU A 124  -28.865  46.255  -2.333  1.00 48.85  A C
ATOM  685  OE1 GLU A 124  -28.046  45.580  -2.996  1.00 50.17  A O
ATOM  686  OE2 GLU A 124  -29.862  46.811  -2.862  1.00 49.28  A O
ATOM  687  C   GLU A 124  -26.327  47.862  -0.348  1.00 41.27  A C
ATOM  688  O   GLU A 124  -26.730  48.466   0.641  1.00 41.61  A O
ATOM  689  N   PRO A 125  -26.068  48.488  -1.502  1.00 40.06  A N
ATOM  690  CD  PRO A 125  -26.402  49.889  -1.813  1.00 39.60  A C
ATOM  691  CA  PRO A 125  -25.557  47.794  -2.685  1.00 39.43  A C
ATOM  692  CB  PRO A 125  -25.821  48.792  -3.806  1.00 39.62  A C
ATOM  693  CG  PRO A 125  -25.662  50.111  -3.106  1.00 39.43  A C
ATOM  694  C   PRO A 125  -24.075  47.480  -2.515  1.00 38.97  A C
ATOM  695  O   PRO A 125  -23.369  48.163  -1.773  1.00 38.90  A O
ATOM  696  N   VAL A 126  -23.614  46.440  -3.197  1.00 38.10  A N
ATOM  697  CA  VAL A 126  -22.219  46.047  -3.108  1.00 37.01  A C
ATOM  698  CB  VAL A 126  -22.004  44.996  -1.997  1.00 37.00  A C
ATOM  699  CG1 VAL A 126  -22.642  43.670  -2.405  1.00 36.38  A C
ATOM  700  CG2 VAL A 126  -20.521  44.820  -1.717  1.00 36.78  A C
ATOM  701  C   VAL A 126  -21.721  45.462  -4.423  1.00 36.45  A C
ATOM  702  O   VAL A 126  -22.506  45.011  -5.262  1.00 36.04  A O
ATOM  703  N   GLN A 127  -20.403  45.478  -4.585  1.00 35.64  A N
ATOM  704  CA  GLN A 127  -19.750  44.940  -5.770  1.00 34.71  A C
ATOM  705  CB  GLN A 127  -19.739  45.974  -6.895  1.00 33.75  A C
ATOM  706  CG  GLN A 127  -19.445  45.380  -8.256  1.00 33.43  A C
ATOM  707  CD  GLN A 127  -19.391  46.420  -9.360  1.00 33.47  A C
ATOM  708  OE1 GLN A 127  -19.526  46.094 -10.540  1.00 33.06  A O
ATOM  709  NE2 GLN A 127  -19.182  47.676  -8.985  1.00 33.86  A N
ATOM  710  C   GLN A 127  -18.319  44.619  -5.364  1.00 34.38  A C
ATOM  711  O   GLN A 127  -17.712  45.375  -4.603  1.00 34.23  A O
ATOM  712  N   ASP A 128  -17.778  43.502  -5.845  1.00 33.87  A N
ATOM  713  CA  ASP A 128  -16.406  43.166  -5.495  1.00 33.29  A C
ATOM  714  CB  ASP A 128  -16.174  41.644  -5.556  1.00 33.89  A C
ATOM  715  CG  ASP A 128  -16.219  41.075  -6.963  1.00 34.07  A C
ATOM  716  OD1 ASP A 128  -16.489  39.861  -7.081  1.00 33.80  A O
ATOM  717  OD2 ASP A 128  -15.968  41.810  -7.940  1.00 34.54  A O
ATOM  718  C   ASP A 128  -15.452  43.937  -6.407  1.00 32.83  A C
ATOM  719  O   ASP A 128  -15.820  44.318  -7.520  1.00 32.76  A O
ATOM  720  N   LEU A 129  -14.241  44.190  -5.921  1.00 31.97  A N
ATOM  721  CA  LEU A 129  -13.251  44.946  -6.674  1.00 30.87  A C
ATOM  722  CB  LEU A 129  -11.949  45.028  -5.876  1.00 30.65  A C
ATOM  723  CG  LEU A 129  -10.874  46.008  -6.362  1.00 30.12  A C
ATOM  724  CD1 LEU A 129  -11.456  47.412  -6.488  1.00 29.34  A C
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FIGURE 3A-14

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ATOM   725  CD2 LEU A 129    -9.714   46.005   -5.381  1.00 29.33   A C
ATOM   726  C   LEU A 129   -12.980   44.390   -8.068  1.00 30.82   A C
ATOM   727  O   LEU A 129   -12.646   45.137   -8.986  1.00 30.41   A O
ATOM   728  N   PHE A 130   -13.130   43.083   -8.235  1.00 31.39   A N
ATOM   729  CA  PHE A 130   -12.891   42.470   -9.536  1.00 31.88   A C
ATOM   730  CB  PHE A 130   -13.014   40.954   -9.447  1.00 32.83   A C
ATOM   731  CG  PHE A 130   -12.681   40.247  -10.730  1.00 33.86   A C
ATOM   732  CD1 PHE A 130   -11.364   39.924  -11.038  1.00 34.05   A C
ATOM   733  CD2 PHE A 130   -13.687   39.913  -11.637  1.00 34.34   A C
ATOM   734  CE1 PHE A 130   -11.049   39.277  -12.228  1.00 34.23   A C
ATOM   735  CE2 PHE A 130   -13.384   39.266  -12.830  1.00 34.36   A C
ATOM   736  CZ  PHE A 130   -12.061   38.946  -13.127  1.00 34.68   A C
ATOM   737  C   PHE A 130   -13.882   42.993  -10.568  1.00 32.15   A C
ATOM   738  O   PHE A 130   -13.489   43.516  -11.611  1.00 32.19   A O
ATOM   739  N   ASP A 131   -15.170   42.849  -10.280  1.00 32.14   A N
ATOM   740  CA  ASP A 131   -16.195   43.319  -11.200  1.00 32.37   A C
ATOM   741  CB  ASP A 131   -17.586   42.933  -10.693  1.00 32.81   A C
ATOM   742  CG  ASP A 131   -17.777   41.436  -10.619  1.00 33.24   A C
ATOM   743  OD1 ASP A 131   -17.240   40.734  -11.505  1.00 33.62   A O
ATOM   744  OD2 ASP A 131   -18.466   40.966   -9.686  1.00 33.02   A O
ATOM   745  C   ASP A 131   -16.119   44.826  -11.399  1.00 32.43   A C
ATOM   746  O   ASP A 131   -16.341   45.325  -12.502  1.00 32.49   A O
ATOM   747  N   PHE A 132   -15.810   45.550  -10.328  1.00 32.84   A N
ATOM   748  CA  PHE A 132   -15.704   47.000  -10.397  1.00 32.97   A C
ATOM   749  CB  PHE A 132   -15.384   47.568   -9.007  1.00 32.67   A C
ATOM   750  CG  PHE A 132   -15.376   49.074   -8.942  1.00 32.70   A C
ATOM   751  CD1 PHE A 132   -14.211   49.794   -9.199  1.00 32.57   A C
ATOM   752  CD2 PHE A 132   -16.531   49.776   -8.606  1.00 32.42   A C
ATOM   753  CE1 PHE A 132   -14.196   51.192   -9.120  1.00 32.35   A C
ATOM   754  CE2 PHE A 132   -16.526   51.171   -8.525  1.00 32.21   A C
ATOM   755  CZ  PHE A 132   -15.355   51.879   -8.781  1.00 32.16   A C
ATOM   756  C   PHE A 132   -14.620   47.376  -11.403  1.00 33.46   A C
ATOM   757  O   PHE A 132   -14.870   48.158  -12.320  1.00 33.70   A O
ATOM   758  N   ILE A 133   -13.429   46.797  -11.250  1.00 33.78   A N
ATOM   759  CA  ILE A 133   -12.307   47.081  -12.148  1.00 34.01   A C
ATOM   760  CB  ILE A 133   -11.006   46.420  -11.631  1.00 33.36   A C
ATOM   761  CG2 ILE A 133    -9.897   46.547  -12.662  1.00 32.84   A C
ATOM   762  CG1 ILE A 133   -10.577   47.091  -10.327  1.00 33.01   A C
ATOM   763  CD1 ILE A 133    -9.326   46.510   -9.707  1.00 33.02   A C
ATOM   764  C   ILE A 133   -12.571   46.626  -13.584  1.00 34.68   A C
ATOM   765  O   ILE A 133   -12.196   47.307  -14.540  1.00 34.81   A O
ATOM   766  N   THR A 134   -13.220   45.476  -13.727  1.00 35.47   A N
ATOM   767  CA  THR A 134   -13.555   44.931  -15.037  1.00 36.48   A C
ATOM   768  CB  THR A 134   -14.245   43.560  -14.903  1.00 36.38   A C
ATOM   769  OG1 THR A 134   -13.359   42.637  -14.259  1.00 37.27   A O
ATOM   770  CG2 THR A 134   -14.630   43.014  -16.270  1.00 36.21   A C
ATOM   771  C   THR A 134   -14.520   45.889  -15.730  1.00 37.17   A C
ATOM   772  O   THR A 134   -14.540   45.997  -16.956  1.00 37.28   A O
ATOM   773  N   GLU A 135   -15.301   46.604  -14.932  1.00 38.50   A N
ATOM   774  CA  GLU A 135   -16.281   47.535  -15.464  1.00 39.61   A C
ATOM   775  CB  GLU A 135   -17.302   47.846  -14.390  1.00 41.18   A C
ATOM   776  CG  GLU A 135   -18.704   47.993  -14.881  1.00 43.78   A C
ATOM   777  CD  GLU A 135   -19.618   47.107  -14.071  1.00 45.84   A C
ATOM   778  OE1 GLU A 135   -19.767   45.918  -14.442  1.00 46.46   A O
ATOM   779  OE2 GLU A 135   -20.196   47.612  -13.072  1.00 47.12   A O
ATOM   780  C   GLU A 135   -15.664   48.844  -15.950  1.00 39.55   A C
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FIGURE 3A-15

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ATOM  781  O   GLU A 135  -15.837  49.239 -17.103  1.00 39.75  A O
ATOM  782  N   ARG A 136  -14.940  49.507 -15.055  1.00 38.81  A N
ATOM  783  CA  ARG A 136  -14.316  50.790 -15.349  1.00 38.32  A C
ATOM  784  CB  ARG A 136  -14.336  51.669 -14.102  1.00 39.53  A C
ATOM  785  CG  ARG A 136  -15.669  51.786 -13.408  1.00 40.80  A C
ATOM  786  CD  ARG A 136  -15.567  52.881 -12.357  1.00 42.79  A C
ATOM  787  NE  ARG A 136  -16.824  53.126 -11.655  1.00 43.60  A N
ATOM  788  CZ  ARG A 136  -17.027  54.155 -10.839  1.00 43.66  A C
ATOM  789  NH1 ARG A 136  -16.054  55.035 -10.627  1.00 43.18  A N
ATOM  790  NH2 ARG A 136  -18.198  54.301 -10.231  1.00 43.84  A N
ATOM  791  C   ARG A 136  -12.880  50.730 -15.845  1.00 37.47  A C
ATOM  792  O   ARG A 136  -12.330  51.753 -16.241  1.00 37.36  A O
ATOM  793  N   GLY A 137  -12.261  49.554 -15.808  1.00 36.50  A N
ATOM  794  CA  GLY A 137  -10.877  49.459 -16.241  1.00 34.82  A C
ATOM  795  C   GLY A 137   -9.964  50.109 -15.210  1.00 33.86  A C
ATOM  796  O   GLY A 137  -10.309  50.182 -14.027  1.00 33.69  A O
ATOM  797  N   ALA A 138   -8.808  50.595 -15.649  1.00 32.62  A N
ATOM  798  CA  ALA A 138   -7.862  51.226 -14.740  1.00 31.43  A C
ATOM  799  CB  ALA A 138   -6.703  51.819 -15.526  1.00 30.83  A C
ATOM  800  C   ALA A 138   -8.532  52.304 -13.891  1.00 30.88  A C
ATOM  801  O   ALA A 138   -9.243  53.164 -14.407  1.00 31.18  A O
ATOM  802  N   LEU A 139   -8.307  52.238 -12.583  1.00 30.21  A N
ATOM  803  CA  LEU A 139   -8.872  53.203 -11.653  1.00 29.62  A C
ATOM  804  CB  LEU A 139   -9.006  52.590 -10.258  1.00 29.01  A C
ATOM  805  CG  LEU A 139   -9.766  51.271 -10.104  1.00 29.60  A C
ATOM  806  CD1 LEU A 139   -9.682  50.809  -8.657  1.00 29.23  A C
ATOM  807  CD2 LEU A 139  -11.216  51.448 -10.529  1.00 29.85  A C
ATOM  808  C   LEU A 139   -7.954  54.414 -11.565  1.00 29.62  A C
ATOM  809  O   LEU A 139   -6.738  54.291 -11.702  1.00 29.07  A O
ATOM  810  N   GLN A 140   -8.539  55.585 -11.345  1.00 29.71  A N
ATOM  811  CA  GLN A 140   -7.757  56.801 -11.204  1.00 30.14  A C
ATOM  812  CB  GLN A 140   -8.669  58.018 -11.093  1.00 31.57  A C
ATOM  813  CG  GLN A 140   -9.322  58.433 -12.393  1.00 34.09  A C
ATOM  814  CD  GLN A 140  -10.351  59.529 -12.189  1.00 35.96  A C
ATOM  815  OE1 GLN A 140  -10.128  60.471 -11.414  1.00 37.35  A O
ATOM  816  NE2 GLN A 140  -11.481  59.422 -12.888  1.00 35.79  A N
ATOM  817  C   GLN A 140   -6.952  56.652  -9.925  1.00 29.78  A C
ATOM  818  O   GLN A 140   -7.416  56.057  -8.954  1.00 29.82  A O
ATOM  819  N   GLU A 141   -5.745  57.196  -9.917  1.00 29.24  A N
ATOM  820  CA  GLU A 141   -4.903  57.076  -8.749  1.00 28.82  A C
ATOM  821  CB  GLU A 141   -3.556  57.745  -9.018  1.00 28.13  A C
ATOM  822  CG  GLU A 141   -2.734  56.898  -9.989  1.00 27.94  A C
ATOM  823  CD  GLU A 141   -1.327  57.395 -10.204  1.00 27.38  A C
ATOM  824  OE1 GLU A 141   -0.679  57.800  -9.220  1.00 27.64  A O
ATOM  825  OE2 GLU A 141   -0.859  57.359 -11.360  1.00 27.40  A O
ATOM  826  C   GLU A 141   -5.535  57.568  -7.458  1.00 28.99  A C
ATOM  827  O   GLU A 141   -5.306  56.986  -6.398  1.00 29.43  A O
ATOM  828  N   GLU A 142   -6.350  58.613  -7.529  1.00 28.80  A N
ATOM  829  CA  GLU A 142   -6.991  59.111  -6.318  1.00 28.51  A C
ATOM  830  CB  GLU A 142   -7.829  60.354  -6.611  1.00 29.94  A C
ATOM  831  CG  GLU A 142   -8.749  60.722  -5.461  1.00 31.87  A C
ATOM  832  CD  GLU A 142   -9.551  61.969  -5.735  1.00 33.74  A C
ATOM  833  OE1 GLU A 142   -8.982  63.076  -5.627  1.00 34.40  A O
ATOM  834  OE2 GLU A 142  -10.750  61.839  -6.065  1.00 34.91  A O
ATOM  835  C   GLU A 142   -7.890  58.047  -5.704  1.00 27.13  A C
ATOM  836  O   GLU A 142   -7.926  57.877  -4.491  1.00 27.18  A O
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FIGURE 3A-16

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ATOM  837  N   LEU A 143   -8.625  57.345  -6.553  1.00 26.11  A N
ATOM  838  CA  LEU A 143   -9.529  56.297  -6.105  1.00 25.39  A C
ATOM  839  CB  LEU A 143  -10.489  55.933  -7.239  1.00 24.93  A C
ATOM  840  CG  LEU A 143  -11.494  54.803  -7.020  1.00 24.21  A C
ATOM  841  CD1 LEU A 143  -12.402  55.126  -5.850  1.00 23.68  A C
ATOM  842  CD2 LEU A 143  -12.294  54.613  -8.288  1.00 23.64  A C
ATOM  843  C   LEU A 143   -8.723  55.073  -5.677  1.00 25.26  A C
ATOM  844  O   LEU A 143   -9.037  54.431  -4.674  1.00 25.34  A O
ATOM  845  N   ALA A 144   -7.681  54.757  -6.444  1.00 24.86  A N
ATOM  846  CA  ALA A 144   -6.818  53.621  -6.132  1.00 24.21  A C
ATOM  847  CB  ALA A 144   -5.742  53.478  -7.190  1.00 23.73  A C
ATOM  848  C   ALA A 144   -6.180  53.839  -4.768  1.00 24.07  A C
ATOM  849  O   ALA A 144   -6.028  52.904  -3.984  1.00 24.37  A O
ATOM  850  N   ARG A 145   -5.813  55.086  -4.491  1.00 23.71  A N
ATOM  851  CA  ARG A 145   -5.193  55.438  -3.223  1.00 23.70  A C
ATOM  852  CB  ARG A 145   -4.748  56.908  -3.244  1.00 23.18  A C
ATOM  853  CG  ARG A 145   -4.252  57.440  -1.911  1.00 22.41  A C
ATOM  854  CD  ARG A 145   -3.305  58.616  -2.091  1.00 22.87  A C
ATOM  855  NE  ARG A 145   -3.868  59.644  -2.959  1.00 23.99  A N
ATOM  856  CZ  ARG A 145   -3.367  59.984  -4.141  1.00 24.00  A C
ATOM  857  NH1 ARG A 145   -2.281  59.384  -4.605  1.00 23.84  A N
ATOM  858  NH2 ARG A 145   -3.960  60.922  -4.866  1.00 24.70  A N
ATOM  859  C   ARG A 145   -6.156  55.192  -2.072  1.00 23.74  A C
ATOM  860  O   ARG A 145   -5.796  54.567  -1.077  1.00 23.98  A O
ATOM  861  N   SER A 146   -7.384  55.682  -2.213  1.00 24.11  A N
ATOM  862  CA  SER A 146   -8.393  55.507  -1.174  1.00 23.88  A C
ATOM  863  CB  SER A 146   -9.690  56.207  -1.571  1.00 24.01  A C
ATOM  864  OG  SER A 146  -10.724  55.906  -0.646  1.00 24.93  A O
ATOM  865  C   SER A 146   -8.672  54.030  -0.925  1.00 23.87  A C
ATOM  866  O   SER A 146   -8.721  53.579   0.220  1.00 23.67  A O
ATOM  867  N   PHE A 147   -8.857  53.278  -2.004  1.00 23.51  A N
ATOM  868  CA  PHE A 147   -9.129  51.856  -1.886  1.00 23.53  A C
ATOM  869  CB  PHE A 147   -9.444  51.254  -3.259  1.00 23.38  A C
ATOM  870  CG  PHE A 147  -10.845  51.522  -3.738  1.00 23.87  A C
ATOM  871  CD1 PHE A 147  -11.312  50.930  -4.906  1.00 24.06  A C
ATOM  872  CD2 PHE A 147  -11.707  52.355  -3.017  1.00 25.10  A C
ATOM  873  CE1 PHE A 147  -12.615  51.156  -5.351  1.00 24.66  A C
ATOM  874  CE2 PHE A 147  -13.017  52.591  -3.453  1.00 24.72  A C
ATOM  875  CZ  PHE A 147  -13.469  51.990  -4.623  1.00 25.15  A C
ATOM  876  C   PHE A 147   -7.944  51.133  -1.268  1.00 23.56  A C
ATOM  877  O   PHE A 147   -8.080  50.455  -0.249  1.00 23.49  A O
ATOM  878  N   PHE A 148   -6.779  51.291  -1.884  1.00 23.69  A N
ATOM  879  CA  PHE A 148   -5.571  50.644  -1.398  1.00 23.74  A C
ATOM  880  CB  PHE A 148   -4.364  51.110  -2.211  1.00 23.23  A C
ATOM  881  CG  PHE A 148   -3.127  50.306  -1.963  1.00 23.38  A C
ATOM  882  CD1 PHE A 148   -3.089  48.954  -2.282  1.00 23.13  A C
ATOM  883  CD2 PHE A 148   -1.999  50.894  -1.400  1.00 23.81  A C
ATOM  884  CE1 PHE A 148   -1.947  48.195  -2.044  1.00 23.27  A C
ATOM  885  CE2 PHE A 148   -0.848  50.142  -1.158  1.00 24.14  A C
ATOM  886  CZ  PHE A 148   -0.825  48.788  -1.482  1.00 23.56  A C
ATOM  887  C   PHE A 148   -5.355  50.945   0.083  1.00 23.91  A C
ATOM  888  O   PHE A 148   -5.032  50.055   0.872  1.00 24.10  A O
ATOM  889  N   TRP A 149   -5.546  52.202   0.463  1.00 24.02  A N
ATOM  890  CA  TRP A 149   -5.377  52.600   1.852  1.00 24.16  A C
ATOM  891  CB  TRP A 149   -5.640  54.098   1.999  1.00 23.86  A C
ATOM  892  CG  TRP A 149   -5.523  54.597   3.401  1.00 23.71  A C
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FIGURE 3A-17

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ATOM  893  CD2 TRP A 149    -4.348  55.120   4.030  1.00 24.07   A C
ATOM  894  CE2 TRP A 149    -4.705  55.478   5.348  1.00 24.16   A C
ATOM  895  CE3 TRP A 149    -3.026  55.326   3.607  1.00 24.88   A C
ATOM  896  CD1 TRP A 149    -6.512  54.649   4.334  1.00 23.75   A C
ATOM  897  NE1 TRP A 149    -6.032  55.177   5.507  1.00 24.08   A N
ATOM  898  CZ2 TRP A 149    -3.789  56.030   6.253  1.00 23.64   A C
ATOM  899  CZ3 TRP A 149    -2.110  55.878   4.510  1.00 24.22   A C
ATOM  900  CH2 TRP A 149    -2.502  56.223   5.816  1.00 23.99   A C
ATOM  901  C   TRP A 149    -6.303  51.810   2.778  1.00 24.61   A C
ATOM  902  O   TRP A 149    -5.880  51.336   3.834  1.00 24.44   A O
ATOM  903  N   GLN A 150    -7.563  51.660   2.385  1.00 24.62   A N
ATOM  904  CA  GLN A 150    -8.502  50.922   3.216  1.00 24.93   A C
ATOM  905  CB  GLN A 150    -9.916  51.028   2.652  1.00 24.65   A C
ATOM  906  CG  GLN A 150   -10.509  52.405   2.820  1.00 24.72   A C
ATOM  907  CD  GLN A 150   -11.945  52.471   2.389  1.00 24.92   A C
ATOM  908  OE1 GLN A 150   -12.796  51.745   2.909  1.00 25.73   A O
ATOM  909  NE2 GLN A 150   -12.233  53.343   1.433  1.00 24.37   A N
ATOM  910  C   GLN A 150    -8.102  49.464   3.363  1.00 25.33   A C
ATOM  911  O   GLN A 150    -8.260  48.880   4.435  1.00 25.92   A O
ATOM  912  N   VAL A 151    -7.587  48.876   2.289  1.00 25.25   A N
ATOM  913  CA  VAL A 151    -7.145  47.488   2.331  1.00 25.03   A C
ATOM  914  CB  VAL A 151    -6.720  47.010   0.922  1.00 24.97   A C
ATOM  915  CG1 VAL A 151    -6.102  45.628   0.990  1.00 24.00   A C
ATOM  916  CG2 VAL A 151    -7.940  46.990   0.006  1.00 24.08   A C
ATOM  917  C   VAL A 151    -5.973  47.390   3.318  1.00 25.35   A C
ATOM  918  O   VAL A 151    -5.902  46.462   4.124  1.00 25.04   A O
ATOM  919  N   LEU A 152    -5.067  48.363   3.263  1.00 25.21   A N
ATOM  920  CA  LEU A 152    -3.927  48.398   4.172  1.00 25.75   A C
ATOM  921  CB  LEU A 152    -3.080  49.643   3.907  1.00 26.75   A C
ATOM  922  CG  LEU A 152    -1.853  49.524   2.998  1.00 27.38   A C
ATOM  923  CD1 LEU A 152    -0.743  48.804   3.745  1.00 28.24   A C
ATOM  924  CD2 LEU A 152    -2.213  48.786   1.724  1.00 27.81   A C
ATOM  925  C   LEU A 152    -4.394  48.404   5.631  1.00 26.06   A C
ATOM  926  O   LEU A 152    -3.864  47.666   6.464  1.00 26.92   A O
ATOM  927  N   GLU A 153    -5.382  49.238   5.943  1.00 25.55   A N
ATOM  928  CA  GLU A 153    -5.894  49.310   7.305  1.00 25.01   A C
ATOM  929  CB  GLU A 153    -6.923  50.436   7.444  1.00 24.91   A C
ATOM  930  CG  GLU A 153    -6.369  51.849   7.299  1.00 24.63   A C
ATOM  931  CD  GLU A 153    -5.447  52.254   8.429  1.00 24.61   A C
ATOM  932  OE1 GLU A 153    -5.860  52.188   9.606  1.00 25.80   A O
ATOM  933  OE2 GLU A 153    -4.305  52.646   8.141  1.00 24.66   A O
ATOM  934  C   GLU A 153    -6.549  47.990   7.676  1.00 24.96   A C
ATOM  935  O   GLU A 153    -6.428  47.522   8.807  1.00 25.02   A O
ATOM  936  N   ALA A 154    -7.245  47.389   6.719  1.00 24.74   A N
ATOM  937  CA  ALA A 154    -7.927  46.121   6.960  1.00 24.40   A C
ATOM  938  CB  ALA A 154    -8.736  45.730   5.734  1.00 23.60   A C
ATOM  939  C   ALA A 154    -6.923  45.019   7.305  1.00 24.50   A C
ATOM  940  O   ALA A 154    -7.065  44.322   8.315  1.00 24.02   A O
ATOM  941  N   VAL A 155    -5.907  44.879   6.458  1.00 24.37   A N
ATOM  942  CA  VAL A 155    -4.871  43.876   6.645  1.00 23.98   A C
ATOM  943  CB  VAL A 155    -3.918  43.868   5.437  1.00 23.74   A C
ATOM  944  CG1 VAL A 155    -2.766  42.906   5.675  1.00 23.12   A C
ATOM  945  CG2 VAL A 155    -4.694  43.471   4.189  1.00 22.23   A C
ATOM  946  C   VAL A 155    -4.087  44.100   7.939  1.00 24.45   A C
ATOM  947  O   VAL A 155    -3.766  43.144   8.646  1.00 24.66   A O
ATOM  948  N   ARG A 156    -3.783  45.355   8.253  1.00 24.87   A N
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FIGURE 3A-18

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ATOM   949  CA  ARG A 156    -3.057  45.664   9.484  1.00 25.73   A C
ATOM   950  CB  ARG A 156    -2.835  47.169   9.620  1.00 25.57   A C
ATOM   951  CG  ARG A 156    -1.757  47.727   8.721  1.00 25.81   A C
ATOM   952  CD  ARG A 156    -1.628  49.217   8.949  1.00 26.16   A C
ATOM   953  NE  ARG A 156    -1.390  49.529  10.355  1.00 25.39   A N
ATOM   954  CZ  ARG A 156    -1.560  50.736  10.888  1.00 25.56   A C
ATOM   955  NH1 ARG A 156    -1.973  51.746  10.129  1.00 25.06   A N
ATOM   956  NH2 ARG A 156    -1.318  50.932  12.178  1.00 24.70   A N
ATOM   957  C   ARG A 156    -3.850  45.174  10.685  1.00 26.21   A C
ATOM   958  O   ARG A 156    -3.286  44.681  11.658  1.00 26.09   A O
ATOM   959  N   HIS A 157    -5.167  45.324  10.605  1.00 27.27   A N
ATOM   960  CA  HIS A 157    -6.060  44.900  11.672  1.00 28.10   A C
ATOM   961  CB  HIS A 157    -7.496  45.314  11.342  1.00 28.83   A C
ATOM   962  CG  HIS A 157    -8.492  44.906  12.381  1.00 29.71   A C
ATOM   963  CD2 HIS A 157    -9.511  44.014  12.339  1.00 29.89   A C
ATOM   964  ND1 HIS A 157    -8.483  45.417  13.661  1.00 29.64   A N
ATOM   965  CE1 HIS A 157    -9.452  44.857  14.362  1.00 30.46   A C
ATOM   966  NE2 HIS A 157   -10.091  44.001  13.584  1.00 30.34   A N
ATOM   967  C   HIS A 157    -5.980  43.385  11.850  1.00 28.43   A C
ATOM   968  O   HIS A 157    -5.838  42.890  12.964  1.00 27.78   A O
ATOM   969  N   CYS A 158    -6.080  42.656  10.743  1.00 28.85   A N
ATOM   970  CA  CYS A 158    -6.002  41.205  10.777  1.00 29.90   A C
ATOM   971  CB  CYS A 158    -6.041  40.629   9.360  1.00 29.92   A C
ATOM   972  SG  CYS A 158    -7.624  40.767   8.518  1.00 30.27   A S
ATOM   973  C   CYS A 158    -4.715  40.754  11.457  1.00 30.90   A C
ATOM   974  O   CYS A 158    -4.754  40.035  12.457  1.00 30.43   A O
ATOM   975  N   HIS A 159    -3.577  41.174  10.903  1.00 31.97   A N
ATOM   976  CA  HIS A 159    -2.274  40.805  11.451  1.00 33.00   A C
ATOM   977  CB  HIS A 159    -1.143  41.488  10.676  1.00 33.25   A C
ATOM   978  CG  HIS A 159    -1.010  41.019   9.260  1.00 33.78   A C
ATOM   979  CD2 HIS A 159    -1.756  40.155   8.531  1.00 33.93   A C
ATOM   980  ND1 HIS A 159     0.005  41.443   8.428  1.00 34.42   A N
ATOM   981  CE1 HIS A 159    -0.121  40.859   7.250  1.00 34.09   A C
ATOM   982  NE2 HIS A 159    -1.181  40.072   7.286  1.00 34.10   A N
ATOM   983  C   HIS A 159    -2.196  41.206  12.908  1.00 33.51   A C
ATOM   984  O   HIS A 159    -1.642  40.492  13.734  1.00 33.68   A O
ATOM   985  N   ASN A 160    -2.768  42.359  13.216  1.00 34.53   A N
ATOM   986  CA  ASN A 160    -2.769  42.870  14.571  1.00 35.45   A C
ATOM   987  CB  ASN A 160    -3.405  44.252  14.584  1.00 36.72   A C
ATOM   988  CG  ASN A 160    -3.126  44.998  15.856  1.00 38.28   A C
ATOM   989  OD1 ASN A 160    -3.716  44.721  16.903  1.00 38.86   A O
ATOM   990  ND2 ASN A 160    -2.205  45.945  15.781  1.00 40.04   A N
ATOM   991  C   ASN A 160    -3.520  41.940  15.522  1.00 35.76   A C
ATOM   992  O   ASN A 160    -3.279  41.950  16.727  1.00 35.78   A O
ATOM   993  N   CME A 161    -4.429  41.140  14.969  1.00 36.10   A N
ATOM   994  CA  CME A 161    -5.226  40.204  15.756  1.00 35.76   A C
ATOM   995  C   CME A 161    -4.751  38.763  15.572  1.00 34.38   A C
ATOM   996  CB  CME A 161    -6.704  40.309  15.365  1.00 37.89   A C
ATOM   997  SG  CME A 161    -7.621  41.814  15.878  1.00 42.07   A S
ATOM   998  S1  CME A 161    -7.310  42.058  17.938  1.00 45.24   A S
ATOM   999  C1  CME A 161    -6.265  43.547  18.187  1.00 45.82   A C
ATOM  1000  C2  CME A 161    -5.721  43.786  19.599  1.00 46.85   A C
ATOM  1001  O1  CME A 161    -6.751  44.150  20.537  1.00 47.93   A O
ATOM  1002  O   CME A 161    -5.466  37.823  15.904  1.00 34.21   A O
ATOM  1003  N   GLY A 162    -3.548  38.597  15.029  1.00 32.70   A N
ATOM  1004  CA  GLY A 162    -2.992  37.269  14.833  1.00 30.82   A C
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FIGURE 3A-19

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ATOM 1005  C   GLY A 162   -3.502  36.490  13.639  1.00 29.85  A C
ATOM 1006  O   GLY A 162   -3.221  35.300  13.514  1.00 29.76  A O
ATOM 1007  N   VAL A 163   -4.234  37.159  12.754  1.00 28.88  A N
ATOM 1008  CA  VAL A 163   -4.800  36.526  11.565  1.00 27.52  A C
ATOM 1009  CB  VAL A 163   -6.288  36.908  11.410  1.00 27.20  A C
ATOM 1010  CG1 VAL A 163   -6.884  36.230  10.190  1.00 26.57  A C
ATOM 1011  CG2 VAL A 163   -7.048  36.541  12.668  1.00 26.27  A C
ATOM 1012  C   VAL A 163   -4.078  36.924  10.277  1.00 27.64  A C
ATOM 1013  O   VAL A 163   -3.790  38.102  10.058  1.00 27.58  A O
ATOM 1014  N   LEU A 164   -3.798  35.942   9.423  1.00 27.28  A N
ATOM 1015  CA  LEU A 164   -3.137  36.195   8.144  1.00 27.55  A C
ATOM 1016  CB  LEU A 164   -1.822  35.418   8.067  1.00 27.47  A C
ATOM 1017  CG  LEU A 164   -0.903  35.729   6.884  1.00 27.86  A C
ATOM 1018  CD1 LEU A 164   -0.329  37.135   7.026  1.00 27.32  A C
ATOM 1019  CD2 LEU A 164    0.219  34.711   6.837  1.00 28.12  A C
ATOM 1020  C   LEU A 164   -4.086  35.722   7.043  1.00 27.66  A C
ATOM 1021  O   LEU A 164   -4.420  34.543   6.983  1.00 28.65  A O
ATOM 1022  N   HIS A 165   -4.521  36.628   6.175  1.00 27.14  A N
ATOM 1023  CA  HIS A 165   -5.462  36.264   5.115  1.00 27.41  A C
ATOM 1024  CB  HIS A 165   -5.946  37.526   4.393  1.00 27.04  A C
ATOM 1025  CG  HIS A 165   -7.145  37.304   3.523  1.00 26.00  A C
ATOM 1026  CD2 HIS A 165   -8.431  37.704   3.661  1.00 25.61  A C
ATOM 1027  ND1 HIS A 165   -7.092  36.583   2.350  1.00 25.86  A N
ATOM 1028  CE1 HIS A 165   -8.294  36.550   1.801  1.00 25.87  A C
ATOM 1029  NE2 HIS A 165   -9.124  37.222   2.577  1.00 25.44  A N
ATOM 1030  C   HIS A 165   -4.935  35.247   4.095  1.00 27.80  A C
ATOM 1031  O   HIS A 165   -5.617  34.276   3.772  1.00 27.85  A O
ATOM 1032  N   ARG A 166   -3.732  35.485   3.584  1.00 28.06  A N
ATOM 1033  CA  ARG A 166   -3.079  34.607   2.614  1.00 28.85  A C
ATOM 1034  CB  ARG A 166   -2.881  33.205   3.204  1.00 28.96  A C
ATOM 1035  CG  ARG A 166   -1.908  33.183   4.372  1.00 30.05  A C
ATOM 1036  CD  ARG A 166   -1.286  31.813   4.591  1.00 30.84  A C
ATOM 1037  NE  ARG A 166   -2.265  30.781   4.920  1.00 31.86  A N
ATOM 1038  CZ  ARG A 166   -1.949  29.510   5.153  1.00 32.15  A C
ATOM 1039  NH1 ARG A 166   -0.680  29.122   5.093  1.00 32.26  A N
ATOM 1040  NH2 ARG A 166   -2.896  28.626   5.439  1.00 31.89  A N
ATOM 1041  C   ARG A 166   -3.696  34.487   1.225  1.00 29.22  A C
ATOM 1042  O   ARG A 166   -3.264  33.652   0.428  1.00 29.30  A O
ATOM 1043  N   ASP A 167   -4.696  35.307   0.920  1.00 29.60  A N
ATOM 1044  CA  ASP A 167   -5.297  35.267  -0.410  1.00 30.19  A C
ATOM 1045  CB  ASP A 167   -6.369  34.175  -0.500  1.00 31.24  A C
ATOM 1046  CG  ASP A 167   -6.885  33.972  -1.927  1.00 32.27  A C
ATOM 1047  OD1 ASP A 167   -6.075  34.032  -2.879  1.00 31.88  A O
ATOM 1048  OD2 ASP A 167   -8.102  33.738  -2.096  1.00 33.01  A O
ATOM 1049  C   ASP A 167   -5.885  36.618  -0.786  1.00 29.94  A C
ATOM 1050  O   ASP A 167   -6.957  36.702  -1.375  1.00 30.11  A O
ATOM 1051  N   ILE A 168   -5.167  37.678  -0.441  1.00 29.49  A N
ATOM 1052  CA  ILE A 168   -5.610  39.024  -0.758  1.00 29.04  A C
ATOM 1053  CB  ILE A 168   -4.668  40.068  -0.136  1.00 28.62  A C
ATOM 1054  CG2 ILE A 168   -5.115  41.467  -0.527  1.00 28.12  A C
ATOM 1055  CG1 ILE A 168   -4.639  39.903   1.383  1.00 27.90  A C
ATOM 1056  CD1 ILE A 168   -3.630  40.792   2.071  1.00 27.24  A C
ATOM 1057  C   ILE A 168   -5.615  39.215  -2.274  1.00 29.41  A C
ATOM 1058  O   ILE A 168   -4.645  38.885  -2.948  1.00 29.32  A O
ATOM 1059  N   LYS A 169   -6.715  39.737  -2.803  1.00 29.95  A N
ATOM 1060  CA  LYS A 169   -6.856  40.003  -4.233  1.00 30.50  A C
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FIGURE 3A-20

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ATOM 1061  CB  LYS A 169    -6.806  38.708  -5.044  1.00 30.68  A C
ATOM 1062  CG  LYS A 169    -7.917  37.729  -4.752  1.00 31.56  A C
ATOM 1063  CD  LYS A 169    -7.821  36.520  -5.668  1.00 31.68  A C
ATOM 1064  CE  LYS A 169    -8.943  35.539  -5.397  1.00 32.81  A C
ATOM 1065  NZ  LYS A 169    -8.951  34.432  -6.388  1.00 33.88  A N
ATOM 1066  C   LYS A 169    -8.181  40.723  -4.462  1.00 31.04  A C
ATOM 1067  O   LYS A 169    -8.994  40.831  -3.542  1.00 30.81  A O
ATOM 1068  N   ASP A 170    -8.409  41.210  -5.678  1.00 31.62  A N
ATOM 1069  CA  ASP A 170    -9.635  41.954  -5.970  1.00 31.91  A C
ATOM 1070  CB  ASP A 170    -9.617  42.494  -7.409  1.00 32.09  A C
ATOM 1071  CG  ASP A 170    -9.363  41.416  -8.442  1.00 32.44  A C
ATOM 1072  OD1 ASP A 170    -9.453  40.218  -8.104  1.00 32.55  A O
ATOM 1073  OD2 ASP A 170    -9.083  41.774  -9.605  1.00 33.13  A O
ATOM 1074  C   ASP A 170   -10.941  41.211  -5.716  1.00 32.04  A C
ATOM 1075  O   ASP A 170   -11.917  41.817  -5.272  1.00 32.35  A O
ATOM 1076  N   GLU A 171   -10.971  39.911  -5.988  1.00 32.22  A N
ATOM 1077  CA  GLU A 171   -12.185  39.134  -5.768  1.00 32.65  A C
ATOM 1078  CB  GLU A 171   -12.010  37.704  -6.275  1.00 34.08  A C
ATOM 1079  CG  GLU A 171   -11.769  37.601  -7.767  1.00 36.63  A C
ATOM 1080  CD  GLU A 171   -11.674  36.162  -8.241  1.00 37.66  A C
ATOM 1081  OE1 GLU A 171   -12.683  35.437  -8.128  1.00 38.54  A O
ATOM 1082  OE2 GLU A 171   -10.591  35.755  -8.720  1.00 38.71  A O
ATOM 1083  C   GLU A 171   -12.585  39.098  -4.296  1.00 32.10  A C
ATOM 1084  O   GLU A 171   -13.772  39.132  -3.974  1.00 32.75  A O
ATOM 1085  N   ASN A 172   -11.601  39.031  -3.405  1.00 31.09  A N
ATOM 1086  CA  ASN A 172   -11.884  38.988  -1.976  1.00 30.05  A C
ATOM 1087  CB  ASN A 172   -10.822  38.168  -1.249  1.00 30.17  A C
ATOM 1088  CG  ASN A 172   -10.752  36.749  -1.756  1.00 30.81  A C
ATOM 1089  OD1 ASN A 172   -11.777  36.148  -2.071  1.00 31.78  A O
ATOM 1090  ND2 ASN A 172    -9.547  36.200  -1.832  1.00 30.68  A N
ATOM 1091  C   ASN A 172   -12.007  40.363  -1.331  1.00 29.26  A C
ATOM 1092  O   ASN A 172   -11.818  40.513  -0.127  1.00 29.36  A O
ATOM 1093  N   ILE A 173   -12.332  41.363  -2.140  1.00 28.28  A N
ATOM 1094  CA  ILE A 173   -12.513  42.717  -1.640  1.00 27.69  A C
ATOM 1095  CB  ILE A 173   -11.395  43.654  -2.134  1.00 27.05  A C
ATOM 1096  CG2 ILE A 173   -11.711  45.088  -1.737  1.00 26.18  A C
ATOM 1097  CG1 ILE A 173   -10.052  43.207  -1.547  1.00 26.76  A C
ATOM 1098  CD1 ILE A 173    -8.858  44.012  -2.031  1.00 26.08  A C
ATOM 1099  C   ILE A 173   -13.868  43.248  -2.109  1.00 27.91  A C
ATOM 1100  O   ILE A 173   -14.119  43.375  -3.312  1.00 27.75  A O
ATOM 1101  N   LEU A 174   -14.739  43.539  -1.148  1.00 27.70  A N
ATOM 1102  CA  LEU A 174   -16.075  44.046  -1.429  1.00 28.50  A C
ATOM 1103  CB  LEU A 174   -17.092  43.388  -0.492  1.00 28.49  A C
ATOM 1104  CG  LEU A 174   -17.783  42.101  -0.957  1.00 28.90  A C
ATOM 1105  CD1 LEU A 174   -16.777  41.148  -1.571  1.00 27.75  A C
ATOM 1106  CD2 LEU A 174   -18.507  41.463   0.225  1.00 27.83  A C
ATOM 1107  C   LEU A 174   -16.144  45.554  -1.260  1.00 29.02  A C
ATOM 1108  O   LEU A 174   -15.508  46.115  -0.368  1.00 29.28  A O
ATOM 1109  N   ILE A 175   -16.926  46.207  -2.113  1.00 29.66  A N
ATOM 1110  CA  ILE A 175   -17.085  47.655  -2.044  1.00 30.43  A C
ATOM 1111  CB  ILE A 175   -16.798  48.327  -3.403  1.00 29.68  A C
ATOM 1112  CG2 ILE A 175   -16.890  49.835  -3.256  1.00 29.27  A C
ATOM 1113  CG1 ILE A 175   -15.413  47.932  -3.915  1.00 29.16  A C
ATOM 1114  CD1 ILE A 175   -15.116  48.459  -5.300  1.00 28.37  A C
ATOM 1115  C   ILE A 175   -18.505  48.054  -1.642  1.00 31.77  A C
ATOM 1116  O   ILE A 175   -19.470  47.753  -2.351  1.00 32.32  A O
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FIGURE 3A-21

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ATOM 1117  N   ASP A 176  -18.638  48.717  -0.498  1.00 32.78  A N
ATOM 1118  CA  ASP A 176  -19.943  49.188  -0.064  1.00 33.45  A C
ATOM 1119  CB  ASP A 176  -19.948  49.464   1.440  1.00 34.50  A C
ATOM 1120  CG  ASP A 176  -21.260  50.065   1.920  1.00 35.90  A C
ATOM 1121  OD1 ASP A 176  -21.466  50.133   3.154  1.00 35.90  A O
ATOM 1122  OD2 ASP A 176  -22.081  50.473   1.065  1.00 36.68  A O
ATOM 1123  C   ASP A 176  -20.121  50.477  -0.856  1.00 33.84  A C
ATOM 1124  O   ASP A 176  -19.639  51.542  -0.466  1.00 33.73  A O
ATOM 1125  N   LEU A 177  -20.800  50.355  -1.989  1.00 34.35  A N
ATOM 1126  CA  LEU A 177  -21.034  51.469  -2.897  1.00 34.94  A C
ATOM 1127  CB  LEU A 177  -21.876  50.977  -4.071  1.00 34.39  A C
ATOM 1128  CG  LEU A 177  -21.190  49.843  -4.833  1.00 34.54  A C
ATOM 1129  CD1 LEU A 177  -22.128  49.281  -5.885  1.00 34.44  A C
ATOM 1130  CD2 LEU A 177  -19.906  50.367  -5.466  1.00 34.05  A C
ATOM 1131  C   LEU A 177  -21.628  52.768  -2.341  1.00 35.39  A C
ATOM 1132  O   LEU A 177  -21.436  53.824  -2.942  1.00 35.44  A O
ATOM 1133  N   ASN A 178  -22.337  52.715  -1.215  1.00 35.79  A N
ATOM 1134  CA  ASN A 178  -22.917  53.941  -0.659  1.00 36.63  A C
ATOM 1135  CB  ASN A 178  -24.241  53.658   0.055  1.00 38.13  A C
ATOM 1136  CG  ASN A 178  -25.328  53.197  -0.891  1.00 39.81  A C
ATOM 1137  OD1 ASN A 178  -25.393  53.628  -2.048  1.00 40.82  A O
ATOM 1138  ND2 ASN A 178  -26.204  52.326  -0.399  1.00 40.44  A N
ATOM 1139  C   ASN A 178  -22.009  54.695   0.303  1.00 36.35  A C
ATOM 1140  O   ASN A 178  -21.968  55.926   0.285  1.00 36.43  A O
ATOM 1141  N   ARG A 179  -21.290  53.964   1.148  1.00 36.08  A N
ATOM 1142  CA  ARG A 179  -20.398  54.592   2.117  1.00 35.54  A C
ATOM 1143  CB  ARG A 179  -20.472  53.848   3.452  1.00 35.72  A C
ATOM 1144  CG  ARG A 179  -21.770  53.099   3.650  1.00 36.53  A C
ATOM 1145  CD  ARG A 179  -22.109  52.894   5.113  1.00 37.40  A C
ATOM 1146  NE  ARG A 179  -22.392  54.165   5.774  1.00 38.64  A N
ATOM 1147  CZ  ARG A 179  -23.242  54.309   6.788  1.00 39.22  A C
ATOM 1148  NH1 ARG A 179  -23.903  53.258   7.263  1.00 39.11  A N
ATOM 1149  NH2 ARG A 179  -23.428  55.506   7.329  1.00 39.52  A N
ATOM 1150  C   ARG A 179  -18.953  54.627   1.621  1.00 35.14  A C
ATOM 1151  O   ARG A 179  -18.092  55.246   2.244  1.00 35.38  A O
ATOM 1152  N   GLY A 180  -18.694  53.963   0.500  1.00 34.44  A N
ATOM 1153  CA  GLY A 180  -17.350  53.943  -0.051  1.00 34.03  A C
ATOM 1154  C   GLY A 180  -16.348  53.237   0.847  1.00 33.47  A C
ATOM 1155  O   GLY A 180  -15.188  53.645   0.947  1.00 32.89  A O
ATOM 1156  N   GLU A 181  -16.797  52.169   1.498  1.00 32.72  A N
ATOM 1157  CA  GLU A 181  -15.937  51.410   2.389  1.00 32.27  A C
ATOM 1158  CB  GLU A 181  -16.592  51.281   3.768  1.00 32.61  A C
ATOM 1159  CG  GLU A 181  -17.169  52.579   4.311  1.00 33.71  A C
ATOM 1160  CD  GLU A 181  -17.585  52.473   5.767  1.00 34.08  A C
ATOM 1161  OE1 GLU A 181  -18.042  51.384   6.181  1.00 34.28  A O
ATOM 1162  OE2 GLU A 181  -17.467  53.485   6.493  1.00 33.93  A O
ATOM 1163  C   GLU A 181  -15.665  50.022   1.823  1.00 31.66  A C
ATOM 1164  O   GLU A 181  -16.565  49.378   1.282  1.00 31.09  A O
ATOM 1165  N   LEU A 182  -14.419  49.568   1.944  1.00 30.96  A N
ATOM 1166  CA  LEU A 182  -14.041  48.243   1.466  1.00 30.07  A C
ATOM 1167  CB  LEU A 182  -12.640  48.267   0.851  1.00 29.41  A C
ATOM 1168  CG  LEU A 182  -12.387  49.165  -0.354  1.00 29.21  A C
ATOM 1169  CD1 LEU A 182  -11.114  48.710  -1.041  1.00 28.62  A C
ATOM 1170  CD2 LEU A 182  -13.547  49.086  -1.325  1.00 29.92  A C
ATOM 1171  C   LEU A 182  -14.058  47.239   2.615  1.00 29.82  A C
ATOM 1172  O   LEU A 182  -13.753  47.582   3.756  1.00 29.25  A O
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FIGURE 3A-22

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ATOM 1173  N   LYS A 183  -14.426  46.001   2.303  1.00 30.07  A N
ATOM 1174  CA  LYS A 183  -14.471  44.927   3.293  1.00 30.71  A C
ATOM 1175  CB  LYS A 183  -15.894  44.372   3.447  1.00 31.45  A C
ATOM 1176  CG  LYS A 183  -16.949  45.362   3.886  1.00 32.60  A C
ATOM 1177  CD  LYS A 183  -16.688  45.848   5.285  1.00 33.53  A C
ATOM 1178  CE  LYS A 183  -17.854  46.658   5.795  1.00 33.79  A C
ATOM 1179  NZ  LYS A 183  -17.534  47.199   7.143  1.00 35.44  A N
ATOM 1180  C   LYS A 183  -13.580  43.804   2.783  1.00 30.21  A C
ATOM 1181  O   LYS A 183  -13.539  43.540   1.586  1.00 30.64  A O
ATOM 1182  N   LEU A 184  -12.879  43.136   3.687  1.00 29.80  A N
ATOM 1183  CA  LEU A 184  -12.013  42.028   3.305  1.00 29.44  A C
ATOM 1184  CB  LEU A 184  -10.772  42.029   4.190  1.00 29.60  A C
ATOM 1185  CG  LEU A 184   -9.542  41.306   3.672  1.00 29.64  A C
ATOM 1186  CD1 LEU A 184   -9.189  41.832   2.289  1.00 29.95  A C
ATOM 1187  CD2 LEU A 184   -8.397  41.525   4.651  1.00 29.57  A C
ATOM 1188  C   LEU A 184  -12.818  40.748   3.519  1.00 29.19  A C
ATOM 1189  O   LEU A 184  -13.404  40.566   4.581  1.00 28.95  A O
ATOM 1190  N   ILE A 185  -12.853  39.862   2.527  1.00 29.26  A N
ATOM 1191  CA  ILE A 185  -13.634  38.636   2.664  1.00 29.41  A C
ATOM 1192  CB  ILE A 185  -14.868  38.643   1.747  1.00 29.37  A C
ATOM 1193  CG2 ILE A 185  -15.717  39.859   2.007  1.00 29.23  A C
ATOM 1194  CG1 ILE A 185  -14.415  38.622   0.288  1.00 28.93  A C
ATOM 1195  CD1 ILE A 185  -15.535  38.392  -0.692  1.00 29.20  A C
ATOM 1196  C   ILE A 185  -12.919  37.331   2.357  1.00 29.93  A C
ATOM 1197  O   ILE A 185  -11.859  37.306   1.736  1.00 29.95  A O
ATOM 1198  N   ASP A 186  -13.554  36.247   2.790  1.00 30.58  A N
ATOM 1199  CA  ASP A 186  -13.089  34.887   2.569  1.00 31.55  A C
ATOM 1200  CB  ASP A 186  -13.116  34.583   1.068  1.00 33.37  A C
ATOM 1201  CG  ASP A 186  -12.992  33.099   0.766  1.00 35.64  A C
ATOM 1202  OD1 ASP A 186  -13.000  32.736  -0.435  1.00 36.97  A O
ATOM 1203  OD2 ASP A 186  -12.888  32.297   1.724  1.00 36.62  A O
ATOM 1204  C   ASP A 186  -11.717  34.554   3.144  1.00 31.24  A C
ATOM 1205  O   ASP A 186  -10.704  34.627   2.449  1.00 30.97  A O
ATOM 1206  N   PHE A 187  -11.697  34.178   4.418  1.00 30.93  A N
ATOM 1207  CA  PHE A 187  -10.456  33.809   5.081  1.00 30.95  A C
ATOM 1208  CB  PHE A 187  -10.475  34.267   6.538  1.00 29.88  A C
ATOM 1209  CG  PHE A 187  -10.340  35.751   6.707  1.00 29.14  A C
ATOM 1210  CD1 PHE A 187  -11.297  36.615   6.192  1.00 29.25  A C
ATOM 1211  CD2 PHE A 187   -9.245  36.287   7.370  1.00 28.76  A C
ATOM 1212  CE1 PHE A 187  -11.162  37.998   6.336  1.00 28.89  A C
ATOM 1213  CE2 PHE A 187   -9.103  37.666   7.518  1.00 28.88  A C
ATOM 1214  CZ  PHE A 187  -10.063  38.522   7.001  1.00 28.47  A C
ATOM 1215  C   PHE A 187  -10.288  32.295   5.017  1.00 31.55  A C
ATOM 1216  O   PHE A 187   -9.692  31.686   5.904  1.00 31.88  A O
ATOM 1217  N   GLY A 188  -10.814  31.697   3.952  1.00 31.94  A N
ATOM 1218  CA  GLY A 188  -10.741  30.257   3.788  1.00 32.52  A C
ATOM 1219  C   GLY A 188   -9.357  29.673   3.585  1.00 32.98  A C
ATOM 1220  O   GLY A 188   -9.158  28.478   3.802  1.00 33.39  A O
ATOM 1221  N   SER A 189   -8.404  30.498   3.164  1.00 33.28  A N
ATOM 1222  CA  SER A 189   -7.036  30.033   2.933  1.00 33.55  A C
ATOM 1223  CB  SER A 189   -6.574  30.424   1.531  1.00 34.37  A C
ATOM 1224  OG  SER A 189   -7.604  30.229   0.577  1.00 36.56  A O
ATOM 1225  C   SER A 189   -6.109  30.675   3.953  1.00 33.58  A C
ATOM 1226  O   SER A 189   -4.887  30.542   3.874  1.00 33.11  A O
ATOM 1227  N   GLY A 190   -6.705  31.378   4.909  1.00 33.85  A N
ATOM 1228  CA  GLY A 190   -5.927  32.055   5.927  1.00 34.60  A C
```

FIGURE 3A-23

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ATOM 1229  C   GLY A 190   -5.216  31.139   6.901  1.00 35.32  A C
ATOM 1230  O   GLY A 190   -5.149  29.921   6.712  1.00 36.21  A O
ATOM 1231  N   ALA A 191   -4.681  31.739   7.957  1.00 35.00  A N
ATOM 1232  CA  ALA A 191   -3.964  30.997   8.982  1.00 34.56  A C
ATOM 1233  CB  ALA A 191   -2.679  30.425   8.403  1.00 34.09  A C
ATOM 1234  C   ALA A 191   -3.641  31.941  10.125  1.00 34.39  A C
ATOM 1235  O   ALA A 191   -3.765  33.162   9.989  1.00 34.69  A O
ATOM 1236  N   LEU A 192   -3.241  31.379  11.258  1.00 33.84  A N
ATOM 1237  CA  LEU A 192   -2.875  32.198  12.397  1.00 33.58  A C
ATOM 1238  CB  LEU A 192   -2.724  31.338  13.646  1.00 33.29  A C
ATOM 1239  CG  LEU A 192   -3.999  30.632  14.100  1.00 33.54  A C
ATOM 1240  CD1 LEU A 192   -3.680  29.682  15.248  1.00 33.49  A C
ATOM 1241  CD2 LEU A 192   -5.032  31.674  14.517  1.00 33.20  A C
ATOM 1242  C   LEU A 192   -1.538  32.813  12.027  1.00 33.83  A C
ATOM 1243  O   LEU A 192   -0.692  32.146  11.438  1.00 34.36  A O
ATOM 1244  N   LEU A 193   -1.347  34.085  12.346  1.00 33.96  A N
ATOM 1245  CA  LEU A 193   -0.088  34.736  12.024  1.00 34.28  A C
ATOM 1246  CB  LEU A 193   -0.199  36.250  12.222  1.00 33.61  A C
ATOM 1247  CG  LEU A 193    1.056  37.054  11.870  1.00 32.92  A C
ATOM 1248  CD1 LEU A 193    1.414  36.840  10.408  1.00 32.28  A C
ATOM 1249  CD2 LEU A 193    0.817  38.527  12.153  1.00 32.72  A C
ATOM 1250  C   LEU A 193    1.028  34.186  12.905  1.00 34.91  A C
ATOM 1251  O   LEU A 193    0.839  33.974  14.106  1.00 35.27  A O
ATOM 1252  N   LYS A 194    2.185  33.945  12.298  1.00 35.05  A N
ATOM 1253  CA  LYS A 194    3.344  33.444  13.023  1.00 35.38  A C
ATOM 1254  CB  LYS A 194    3.417  31.913  12.938  1.00 35.29  A C
ATOM 1255  CG  LYS A 194    3.721  31.362  11.554  1.00 35.20  A C
ATOM 1256  CD  LYS A 194    3.690  29.840  11.542  1.00 35.06  A C
ATOM 1257  CE  LYS A 194    3.960  29.299  10.146  1.00 35.23  A C
ATOM 1258  NZ  LYS A 194    3.866  27.816  10.078  1.00 35.01  A N
ATOM 1259  C   LYS A 194    4.587  34.074  12.399  1.00 35.86  A C
ATOM 1260  O   LYS A 194    4.539  34.553  11.263  1.00 35.94  A O
ATOM 1261  N   ASP A 195    5.695  34.084  13.137  1.00 36.23  A N
ATOM 1262  CA  ASP A 195    6.930  34.671  12.631  1.00 36.25  A C
ATOM 1263  CB  ASP A 195    7.670  35.376  13.760  1.00 36.74  A C
ATOM 1264  CG  ASP A 195    6.934  36.598  14.253  1.00 37.34  A C
ATOM 1265  OD1 ASP A 195    6.777  37.556  13.465  1.00 38.25  A O
ATOM 1266  OD2 ASP A 195    6.506  36.602  15.424  1.00 37.54  A O
ATOM 1267  C   ASP A 195    7.848  33.660  11.963  1.00 36.26  A C
ATOM 1268  O   ASP A 195    8.818  34.037  11.307  1.00 36.01  A O
ATOM 1269  N   THR A 196    7.543  32.377  12.129  1.00 36.18  A N
ATOM 1270  CA  THR A 196    8.346  31.329  11.517  1.00 36.41  A C
ATOM 1271  CB  THR A 196    8.254  30.022  12.317  1.00 36.80  A C
ATOM 1272  OG1 THR A 196    6.885  29.621  12.427  1.00 37.51  A O
ATOM 1273  CG2 THR A 196    8.829  30.221  13.712  1.00 37.11  A C
ATOM 1274  C   THR A 196    7.866  31.094  10.089  1.00 36.54  A C
ATOM 1275  O   THR A 196    6.837  31.627   9.681  1.00 36.75  A O
ATOM 1276  N   VAL A 197    8.608  30.292   9.333  1.00 36.68  A N
ATOM 1277  CA  VAL A 197    8.275  30.016   7.938  1.00 36.71  A C
ATOM 1278  CB  VAL A 197    9.408  29.217   7.259  1.00 37.15  A C
ATOM 1279  CG1 VAL A 197    9.537  27.848   7.910  1.00 36.96  A C
ATOM 1280  CG2 VAL A 197    9.137  29.081   5.762  1.00 37.24  A C
ATOM 1281  C   VAL A 197    6.963  29.275   7.687  1.00 36.99  A C
ATOM 1282  O   VAL A 197    6.480  28.515   8.529  1.00 37.75  A O
ATOM 1283  N   TYR A 198    6.396  29.517   6.507  1.00 36.88  A N
ATOM 1284  CA  TYR A 198    5.157  28.884   6.061  1.00 36.68  A C
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FIGURE 3A-24

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ATOM 1285  CB  TYR A 198     4.168  29.943   5.567  1.00 34.64  A C
ATOM 1286  CG  TYR A 198     3.373  30.631   6.654  1.00 32.83  A C
ATOM 1287  CD1 TYR A 198     2.233  30.037   7.192  1.00 31.86  A C
ATOM 1288  CE1 TYR A 198     1.485  30.671   8.183  1.00 31.09  A C
ATOM 1289  CD2 TYR A 198     3.752  31.884   7.136  1.00 31.97  A C
ATOM 1290  CE2 TYR A 198     3.014  32.528   8.130  1.00 31.11  A C
ATOM 1291  CZ  TYR A 198     1.881  31.914   8.647  1.00 30.99  A C
ATOM 1292  OH  TYR A 198     1.157  32.540   9.634  1.00 30.01  A O
ATOM 1293  C   TYR A 198     5.535  27.962   4.902  1.00 37.66  A C
ATOM 1294  O   TYR A 198     6.197  28.391   3.956  1.00 38.18  A O
ATOM 1295  N   THR A 199     5.123  26.702   4.971  1.00 38.53  A N
ATOM 1296  CA  THR A 199     5.449  25.749   3.918  1.00 39.50  A C
ATOM 1297  CB  THR A 199     6.136  24.501   4.489  1.00 39.43  A C
ATOM 1298  OG1 THR A 199     5.300  23.908   5.491  1.00 39.58  A O
ATOM 1299  CG2 THR A 199     7.477  24.870   5.095  1.00 39.56  A C
ATOM 1300  C   THR A 199     4.226  25.301   3.139  1.00 40.54  A C
ATOM 1301  O   THR A 199     4.334  24.482   2.230  1.00 40.80  A O
ATOM 1302  N   ASP A 200     3.064  25.832   3.504  1.00 41.79  A N
ATOM 1303  CA  ASP A 200     1.818  25.490   2.821  1.00 42.62  A C
ATOM 1304  CB  ASP A 200     0.823  24.852   3.792  1.00 43.95  A C
ATOM 1305  CG  ASP A 200     0.357  25.820   4.871  1.00 45.02  A C
ATOM 1306  OD1 ASP A 200     1.202  26.253   5.685  1.00 45.44  A O
ATOM 1307  OD2 ASP A 200    -0.851  26.149   4.902  1.00 45.50  A O
ATOM 1308  C   ASP A 200     1.193  26.749   2.243  1.00 42.59  A C
ATOM 1309  O   ASP A 200     1.311  27.829   2.819  1.00 42.85  A O
ATOM 1310  N   PHE A 201     0.527  26.608   1.106  1.00 42.13  A N
ATOM 1311  CA  PHE A 201    -0.124  27.743   0.477  1.00 41.91  A C
ATOM 1312  CB  PHE A 201     0.891  28.579  -0.304  1.00 41.20  A C
ATOM 1313  CG  PHE A 201     0.285  29.757  -1.010  1.00 40.35  A C
ATOM 1314  CD1 PHE A 201    -0.009  29.696  -2.364  1.00 39.91  A C
ATOM 1315  CD2 PHE A 201    -0.017  30.921  -0.311  1.00 40.09  A C
ATOM 1316  CE1 PHE A 201    -0.596  30.777  -3.012  1.00 40.13  A C
ATOM 1317  CE2 PHE A 201    -0.603  32.006  -0.949  1.00 39.80  A C
ATOM 1318  CZ  PHE A 201    -0.893  31.935  -2.300  1.00 39.96  A C
ATOM 1319  C   PHE A 201    -1.241  27.277  -0.443  1.00 42.39  A C
ATOM 1320  O   PHE A 201    -1.026  26.478  -1.350  1.00 42.47  A O
ATOM 1321  N   ASP A 202    -2.439  27.788  -0.200  1.00 43.12  A N
ATOM 1322  CA  ASP A 202    -3.595  27.415  -0.992  1.00 43.97  A C
ATOM 1323  CB  ASP A 202    -4.554  26.595  -0.131  1.00 45.11  A C
ATOM 1324  CG  ASP A 202    -5.655  25.956  -0.940  1.00 46.25  A C
ATOM 1325  OD1 ASP A 202    -6.647  25.504  -0.329  1.00 47.27  A O
ATOM 1326  OD2 ASP A 202    -5.523  25.898  -2.184  1.00 46.39  A O
ATOM 1327  C   ASP A 202    -4.306  28.657  -1.521  1.00 43.96  A C
ATOM 1328  O   ASP A 202    -5.534  28.693  -1.610  1.00 44.11  A O
ATOM 1329  N   GLY A 203    -3.529  29.677  -1.867  1.00 43.79  A N
ATOM 1330  CA  GLY A 203    -4.112  30.903  -2.378  1.00 42.96  A C
ATOM 1331  C   GLY A 203    -4.044  30.984  -3.889  1.00 42.45  A C
ATOM 1332  O   GLY A 203    -3.849  29.971  -4.560  1.00 43.00  A O
ATOM 1333  N   THR A 204    -4.199  32.192  -4.423  1.00 41.47  A N
ATOM 1334  CA  THR A 204    -4.165  32.413  -5.861  1.00 40.29  A C
ATOM 1335  CB  THR A 204    -4.879  33.724  -6.221  1.00 39.78  A C
ATOM 1336  OG1 THR A 204    -6.166  33.752  -5.593  1.00 38.97  A O
ATOM 1337  CG2 THR A 204    -5.055  33.838  -7.728  1.00 39.77  A C
ATOM 1338  C   THR A 204    -2.720  32.482  -6.335  1.00 40.25  A C
ATOM 1339  O   THR A 204    -1.974  33.379  -5.937  1.00 40.50  A O
ATOM 1340  N   ARG A 205    -2.329  31.545  -7.194  1.00 39.52  A N
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FIGURE 3A-25

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ATOM 1341  CA  ARG A 205    -0.956  31.492  -7.689  1.00 39.15  A C
ATOM 1342  CB  ARG A 205    -0.807  30.392  -8.746  1.00 39.62  A C
ATOM 1343  CG  ARG A 205     0.645  29.962  -8.967  1.00 40.10  A C
ATOM 1344  CD  ARG A 205     0.751  28.750  -9.889  1.00 40.22  A C
ATOM 1345  NE  ARG A 205     2.133  28.293 -10.050  1.00 40.09  A N
ATOM 1346  CZ  ARG A 205     2.856  27.725  -9.089  1.00 39.62  A C
ATOM 1347  NH1 ARG A 205     2.334  27.533  -7.885  1.00 40.08  A N
ATOM 1348  NH2 ARG A 205     4.105  27.351  -9.329  1.00 38.81  A N
ATOM 1349  C   ARG A 205    -0.413  32.809  -8.244  1.00 38.25  A C
ATOM 1350  O   ARG A 205     0.615  33.297  -7.777  1.00 38.47  A O
ATOM 1351  N   VAL A 206    -1.090  33.386  -9.233  1.00 37.18  A N
ATOM 1352  CA  VAL A 206    -0.622  34.640  -9.823  1.00 35.71  A C
ATOM 1353  CB  VAL A 206    -1.572  35.140 -10.940  1.00 35.29  A C
ATOM 1354  CG1 VAL A 206    -1.529  34.184 -12.121  1.00 34.25  A C
ATOM 1355  CG2 VAL A 206    -2.989  35.278 -10.404  1.00 34.96  A C
ATOM 1356  C   VAL A 206    -0.434  35.760  -8.799  1.00 35.21  A C
ATOM 1357  O   VAL A 206     0.142  36.803  -9.117  1.00 34.51  A O
ATOM 1358  N   TYR A 207    -0.921  35.544  -7.576  1.00 34.63  A N
ATOM 1359  CA  TYR A 207    -0.782  36.529  -6.501  1.00 34.20  A C
ATOM 1360  CB  TYR A 207    -2.119  36.754  -5.776  1.00 34.52  A C
ATOM 1361  CG  TYR A 207    -3.036  37.791  -6.401  1.00 34.96  A C
ATOM 1362  CD1 TYR A 207    -3.834  37.485  -7.506  1.00 34.66  A C
ATOM 1363  CE1 TYR A 207    -4.686  38.436  -8.065  1.00 34.65  A C
ATOM 1364  CD2 TYR A 207    -3.112  39.080  -5.874  1.00 35.47  A C
ATOM 1365  CE2 TYR A 207    -3.958  40.039  -6.426  1.00 35.57  A C
ATOM 1366  CZ  TYR A 207    -4.745  39.711  -7.520  1.00 35.68  A C
ATOM 1367  OH  TYR A 207    -5.595  40.662  -8.051  1.00 36.14  A O
ATOM 1368  C   TYR A 207     0.262  36.073  -5.478  1.00 33.78  A C
ATOM 1369  O   TYR A 207     0.526  36.775  -4.498  1.00 32.88  A O
ATOM 1370  N   SER A 208     0.846  34.896  -5.708  1.00 33.57  A N
ATOM 1371  CA  SER A 208     1.855  34.346  -4.799  1.00 33.74  A C
ATOM 1372  CB  SER A 208     1.871  32.821  -4.874  1.00 33.93  A C
ATOM 1373  OG  SER A 208     2.313  32.381  -6.143  1.00 36.03  A O
ATOM 1374  C   SER A 208     3.245  34.890  -5.114  1.00 33.18  A C
ATOM 1375  O   SER A 208     3.560  35.190  -6.266  1.00 33.48  A O
ATOM 1376  N   PRO A 209     4.096  35.019  -4.087  1.00 32.39  A N
ATOM 1377  CD  PRO A 209     3.786  34.712  -2.679  1.00 31.88  A C
ATOM 1378  CA  PRO A 209     5.462  35.532  -4.211  1.00 32.26  A C
ATOM 1379  CB  PRO A 209     5.807  35.900  -2.776  1.00 32.19  A C
ATOM 1380  CG  PRO A 209     5.146  34.812  -2.013  1.00 31.62  A C
ATOM 1381  C   PRO A 209     6.480  34.567  -4.815  1.00 32.59  A C
ATOM 1382  O   PRO A 209     6.285  33.354  -4.813  1.00 32.26  A O
ATOM 1383  N   PRO A 210     7.595  35.108  -5.329  1.00 33.17  A N
ATOM 1384  CD  PRO A 210     7.902  36.550  -5.361  1.00 33.09  A C
ATOM 1385  CA  PRO A 210     8.680  34.339  -5.947  1.00 33.07  A C
ATOM 1386  CB  PRO A 210     9.737  35.403  -6.225  1.00 33.11  A C
ATOM 1387  CG  PRO A 210     8.932  36.629  -6.457  1.00 33.44  A C
ATOM 1388  C   PRO A 210     9.212  33.237  -5.033  1.00 33.28  A C
ATOM 1389  O   PRO A 210     9.562  32.152  -5.494  1.00 33.25  A O
ATOM 1390  N   GLU A 211     9.278  33.530  -3.737  1.00 33.69  A N
ATOM 1391  CA  GLU A 211     9.776  32.570  -2.762  1.00 33.92  A C
ATOM 1392  CB  GLU A 211     9.918  33.220  -1.380  1.00 33.90  A C
ATOM 1393  CG  GLU A 211     8.636  33.821  -0.829  1.00 34.48  A C
ATOM 1394  CD  GLU A 211     8.476  35.298  -1.159  1.00 34.06  A C
ATOM 1395  OE1 GLU A 211     8.994  35.745  -2.202  1.00 33.69  A O
ATOM 1396  OE2 GLU A 211     7.815  36.010  -0.377  1.00 34.17  A O
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FIGURE 3A-26

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ATOM 1397  C   GLU A 211     8.874  31.350  -2.666  1.00 34.44   A C
ATOM 1398  O   GLU A 211     9.355  30.251  -2.426  1.00 34.78   A O
ATOM 1399  N   TRP A 212     7.570  31.533  -2.851  1.00 35.20   A N
ATOM 1400  CA  TRP A 212     6.656  30.398  -2.784  1.00 36.33   A C
ATOM 1401  CB  TRP A 212     5.195  30.844  -2.747  1.00 35.94   A C
ATOM 1402  CG  TRP A 212     4.270  29.696  -3.028  1.00 35.39   A C
ATOM 1403  CD2 TRP A 212     4.048  28.556  -2.192  1.00 35.28   A C
ATOM 1404  CE2 TRP A 212     3.184  27.683  -2.893  1.00 35.01   A C
ATOM 1405  CE3 TRP A 212     4.500  28.181  -0.919  1.00 35.13   A C
ATOM 1406  CD1 TRP A 212     3.548  29.480  -4.168  1.00 35.57   A C
ATOM 1407  NE1 TRP A 212     2.893  28.272  -4.094  1.00 35.48   A N
ATOM 1408  CZ2 TRP A 212     2.762  26.463  -2.362  1.00 34.27   A C
ATOM 1409  CZ3 TRP A 212     4.078  26.962  -0.392  1.00 34.91   A C
ATOM 1410  CH2 TRP A 212     3.219  26.120  -1.116  1.00 34.22   A C
ATOM 1411  C   TRP A 212     6.837  29.489  -3.982  1.00 37.36   A C
ATOM 1412  O   TRP A 212     6.890  28.267  -3.851  1.00 37.73   A O
ATOM 1413  N   ILE A 213     6.914  30.103  -5.153  1.00 38.41   A N
ATOM 1414  CA  ILE A 213     7.072  29.377  -6.400  1.00 39.44   A C
ATOM 1415  CB  ILE A 213     6.856  30.337  -7.586  1.00 39.25   A C
ATOM 1416  CG2 ILE A 213     7.181  29.650  -8.899  1.00 39.18   A C
ATOM 1417  CG1 ILE A 213     5.403  30.823  -7.569  1.00 39.32   A C
ATOM 1418  CD1 ILE A 213     5.074  31.834  -8.629  1.00 40.07   A C
ATOM 1419  C   ILE A 213     8.428  28.679  -6.516  1.00 40.33   A C
ATOM 1420  O   ILE A 213     8.513  27.567  -7.029  1.00 40.43   A O
ATOM 1421  N   ARG A 214     9.479  29.319  -6.017  1.00 41.58   A N
ATOM 1422  CA  ARG A 214    10.825  28.753  -6.087  1.00 42.72   A C
ATOM 1423  CB  ARG A 214    11.863  29.880  -6.204  1.00 43.82   A C
ATOM 1424  CG  ARG A 214    12.109  30.357  -7.629  1.00 45.75   A C
ATOM 1425  CD  ARG A 214    12.588  31.805  -7.679  1.00 47.41   A C
ATOM 1426  NE  ARG A 214    13.881  32.039  -7.034  1.00 48.90   A N
ATOM 1427  CZ  ARG A 214    15.046  31.571  -7.476  1.00 49.68   A C
ATOM 1428  NH1 ARG A 214    15.096  30.827  -8.576  1.00 49.70   A N
ATOM 1429  NH2 ARG A 214    16.167  31.872  -6.830  1.00 49.84   A N
ATOM 1430  C   ARG A 214    11.229  27.828  -4.940  1.00 42.83   A C
ATOM 1431  O   ARG A 214    12.064  26.946  -5.131  1.00 43.32   A O
ATOM 1432  N   TYR A 215    10.653  28.012  -3.754  1.00 42.60   A N
ATOM 1433  CA  TYR A 215    11.033  27.172  -2.620  1.00 42.25   A C
ATOM 1434  CB  TYR A 215    12.023  27.919  -1.726  1.00 42.12   A C
ATOM 1435  CG  TYR A 215    13.095  28.673  -2.472  1.00 42.41   A C
ATOM 1436  CD1 TYR A 215    13.996  28.011  -3.305  1.00 42.62   A C
ATOM 1437  CE1 TYR A 215    14.987  28.711  -3.993  1.00 42.85   A C
ATOM 1438  CD2 TYR A 215    13.212  30.057  -2.343  1.00 42.69   A C
ATOM 1439  CE2 TYR A 215    14.197  30.765  -3.022  1.00 42.53   A C
ATOM 1440  CZ  TYR A 215    15.079  30.089  -3.845  1.00 42.62   A C
ATOM 1441  OH  TYR A 215    16.044  30.795  -4.520  1.00 42.87   A O
ATOM 1442  C   TYR A 215     9.880  26.696  -1.748  1.00 42.11   A C
ATOM 1443  O   TYR A 215    10.108  26.058  -0.725  1.00 42.15   A O
ATOM 1444  N   HIS A 216     8.650  26.993  -2.140  1.00 42.09   A N
ATOM 1445  CA  HIS A 216     7.507  26.600  -1.328  1.00 42.37   A C
ATOM 1446  CB  HIS A 216     7.257  25.094  -1.425  1.00 43.08   A C
ATOM 1447  CG  HIS A 216     6.530  24.681  -2.667  1.00 44.58   A C
ATOM 1448  CD2 HIS A 216     6.490  25.232  -3.904  1.00 45.23   A C
ATOM 1449  ND1 HIS A 216     5.729  23.560  -2.722  1.00 45.32   A N
ATOM 1450  CE1 HIS A 216     5.226  23.439  -3.938  1.00 45.39   A C
ATOM 1451  NE2 HIS A 216     5.673  24.441  -4.675  1.00 45.62   A N
ATOM 1452  C   HIS A 216     7.742  26.997   0.129  1.00 41.93   A C
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FIGURE 3A-27

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ATOM 1453  O   HIS A 216    7.442  26.243   1.052  1.00 42.06  A O
ATOM 1454  N   ARG A 217    8.297  28.189   0.318  1.00 41.27  A N
ATOM 1455  CA  ARG A 217    8.579  28.729   1.643  1.00 40.71  A C
ATOM 1456  CB  ARG A 217   10.037  28.460   2.038  1.00 41.09  A C
ATOM 1457  CG  ARG A 217   10.389  26.995   2.239  1.00 41.92  A C
ATOM 1458  CD  ARG A 217   11.901  26.792   2.297  1.00 41.89  A C
ATOM 1459  NE  ARG A 217   12.530  27.480   3.422  1.00 42.21  A N
ATOM 1460  CZ  ARG A 217   12.410  27.111   4.694  1.00 42.04  A C
ATOM 1461  NH1 ARG A 217   11.678  26.054   5.014  1.00 42.34  A N
ATOM 1462  NH2 ARG A 217   13.029  27.796   5.646  1.00 41.94  A N
ATOM 1463  C   ARG A 217    8.348  30.235   1.589  1.00 40.16  A C
ATOM 1464  O   ARG A 217    8.715  30.892   0.610  1.00 40.52  A O
ATOM 1465  N   TYR A 218    7.735  30.782   2.633  1.00 38.90  A N
ATOM 1466  CA  TYR A 218    7.484  32.217   2.688  1.00 37.27  A C
ATOM 1467  CB  TYR A 218    6.374  32.607   1.700  1.00 36.64  A C
ATOM 1468  CG  TYR A 218    5.005  32.091   2.075  1.00 35.71  A C
ATOM 1469  CD1 TYR A 218    4.218  32.758   3.014  1.00 35.45  A C
ATOM 1470  CE1 TYR A 218    2.975  32.261   3.398  1.00 34.89  A C
ATOM 1471  CD2 TYR A 218    4.512  30.911   1.523  1.00 35.74  A C
ATOM 1472  CE2 TYR A 218    3.270  30.404   1.900  1.00 35.28  A C
ATOM 1473  CZ  TYR A 218    2.509  31.083   2.838  1.00 35.06  A C
ATOM 1474  OH  TYR A 218    1.292  30.577   3.226  1.00 35.19  A O
ATOM 1475  C   TYR A 218    7.093  32.629   4.100  1.00 36.52  A C
ATOM 1476  O   TYR A 218    6.680  31.801   4.914  1.00 36.65  A O
ATOM 1477  N   HIS A 219    7.240  33.912   4.391  1.00 35.39  A N
ATOM 1478  CA  HIS A 219    6.878  34.421   5.698  1.00 34.44  A C
ATOM 1479  CB  HIS A 219    8.044  35.198   6.310  1.00 34.82  A C
ATOM 1480  CG  HIS A 219    9.128  34.316   6.846  1.00 34.67  A C
ATOM 1481  CD2 HIS A 219    9.616  34.163   8.100  1.00 34.88  A C
ATOM 1482  ND1 HIS A 219    9.812  33.417   6.058  1.00 34.80  A N
ATOM 1483  CE1 HIS A 219   10.673  32.747   6.802  1.00 34.46  A C
ATOM 1484  NE2 HIS A 219   10.575  33.180   8.045  1.00 34.36  A N
ATOM 1485  C   HIS A 219    5.646  35.295   5.548  1.00 33.68  A C
ATOM 1486  O   HIS A 219    5.489  35.990   4.553  1.00 33.27  A O
ATOM 1487  N   GLY A 220    4.772  35.237   6.545  1.00 32.98  A N
ATOM 1488  CA  GLY A 220    3.525  35.981   6.522  1.00 32.54  A C
ATOM 1489  C   GLY A 220    3.517  37.425   6.050  1.00 32.42  A C
ATOM 1490  O   GLY A 220    3.071  37.712   4.940  1.00 32.35  A O
ATOM 1491  N   ARG A 221    3.984  38.346   6.885  1.00 32.23  A N
ATOM 1492  CA  ARG A 221    3.972  39.754   6.515  1.00 31.94  A C
ATOM 1493  CB  ARG A 221    4.731  40.558   7.555  1.00 34.19  A C
ATOM 1494  CG  ARG A 221    3.815  41.306   8.465  1.00 37.69  A C
ATOM 1495  CD  ARG A 221    3.935  40.895   9.914  1.00 40.26  A C
ATOM 1496  NE  ARG A 221    3.043  41.750  10.688  1.00 43.45  A N
ATOM 1497  CZ  ARG A 221    2.757  41.591  11.974  1.00 44.83  A C
ATOM 1498  NH1 ARG A 221    3.292  40.590  12.666  1.00 45.59  A N
ATOM 1499  NH2 ARG A 221    1.939  42.451  12.571  1.00 45.09  A N
ATOM 1500  C   ARG A 221    4.516  40.079   5.127  1.00 30.70  A C
ATOM 1501  O   ARG A 221    3.896  40.821   4.368  1.00 29.95  A O
ATOM 1502  N   SER A 222    5.678  39.532   4.799  1.00 29.24  A N
ATOM 1503  CA  SER A 222    6.306  39.808   3.516  1.00 28.54  A C
ATOM 1504  CB  SER A 222    7.737  39.273   3.530  1.00 28.50  A C
ATOM 1505  OG  SER A 222    7.751  37.885   3.788  1.00 29.70  A O
ATOM 1506  C   SER A 222    5.534  39.259   2.307  1.00 27.85  A C
ATOM 1507  O   SER A 222    5.424  39.927   1.280  1.00 28.05  A O
ATOM 1508  N   ALA A 223    5.000  38.049   2.413  1.00 26.48  A N
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FIGURE 3A-28

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ATOM 1509  CA  ALA A 223     4.245  37.490   1.298  1.00 25.60  A C
ATOM 1510  CB  ALA A 223     3.899  36.031   1.565  1.00 25.38  A C
ATOM 1511  C   ALA A 223     2.972  38.304   1.106  1.00 24.96  A C
ATOM 1512  O   ALA A 223     2.454  38.406  -0.007  1.00 24.36  A O
ATOM 1513  N   ALA A 224     2.480  38.886   2.200  1.00 24.30  A N
ATOM 1514  CA  ALA A 224     1.270  39.702   2.169  1.00 24.04  A C
ATOM 1515  CB  ALA A 224     0.814  40.002   3.581  1.00 23.74  A C
ATOM 1516  C   ALA A 224     1.527  41.006   1.416  1.00 24.12  A C
ATOM 1517  O   ALA A 224     0.679  41.475   0.652  1.00 24.32  A O
ATOM 1518  N   VAL A 225     2.701  41.589   1.639  1.00 23.62  A N
ATOM 1519  CA  VAL A 225     3.078  42.829   0.976  1.00 23.17  A C
ATOM 1520  CB  VAL A 225     4.433  43.355   1.514  1.00 23.08  A C
ATOM 1521  CG1 VAL A 225     4.945  44.488   0.640  1.00 22.31  A C
ATOM 1522  CG2 VAL A 225     4.265  43.832   2.952  1.00 22.36  A C
ATOM 1523  C   VAL A 225     3.182  42.597  -0.528  1.00 23.51  A C
ATOM 1524  O   VAL A 225     2.798  43.456  -1.325  1.00 24.00  A O
ATOM 1525  N   TRP A 226     3.700  41.433  -0.916  1.00 23.10  A N
ATOM 1526  CA  TRP A 226     3.836  41.110  -2.332  1.00 22.42  A C
ATOM 1527  CB  TRP A 226     4.553  39.762  -2.519  1.00 22.80  A C
ATOM 1528  CG  TRP A 226     4.504  39.258  -3.940  1.00 22.67  A C
ATOM 1529  CD2 TRP A 226     5.503  39.439  -4.951  1.00 22.39  A C
ATOM 1530  CE2 TRP A 226     5.004  38.865  -6.141  1.00 22.58  A C
ATOM 1531  CE3 TRP A 226     6.772  40.033  -4.968  1.00 22.76  A C
ATOM 1532  CD1 TRP A 226     3.468  38.596  -4.543  1.00 22.71  A C
ATOM 1533  NE1 TRP A 226     3.761  38.358  -5.864  1.00 22.77  A N
ATOM 1534  CZ2 TRP A 226     5.730  38.866  -7.335  1.00 22.72  A C
ATOM 1535  CZ3 TRP A 226     7.493  40.034  -6.157  1.00 22.63  A C
ATOM 1536  CH2 TRP A 226     6.969  39.453  -7.323  1.00 22.84  A C
ATOM 1537  C   TRP A 226     2.471  41.070  -3.015  1.00 21.68  A C
ATOM 1538  O   TRP A 226     2.288  41.651  -4.083  1.00 21.46  A O
ATOM 1539  N   SER A 227     1.517  40.376  -2.403  1.00 21.15  A N
ATOM 1540  CA  SER A 227     0.187  40.294  -2.979  1.00 21.14  A C
ATOM 1541  CB  SER A 227    -0.701  39.358  -2.158  1.00 20.44  A C
ATOM 1542  OG  SER A 227    -0.784  39.778  -0.813  1.00 21.14  A O
ATOM 1543  C   SER A 227    -0.416  41.692  -3.041  1.00 21.22  A C
ATOM 1544  O   SER A 227    -1.153  42.016  -3.971  1.00 21.57  A O
ATOM 1545  N   LEU A 228    -0.102  42.525  -2.054  1.00 21.19  A N
ATOM 1546  CA  LEU A 228    -0.612  43.889  -2.055  1.00 21.17  A C
ATOM 1547  CB  LEU A 228    -0.267  44.598  -0.744  1.00 20.60  A C
ATOM 1548  CG  LEU A 228    -1.096  44.141   0.461  1.00 20.31  A C
ATOM 1549  CD1 LEU A 228    -0.554  44.781   1.733  1.00 19.66  A C
ATOM 1550  CD2 LEU A 228    -2.560  44.509   0.243  1.00 19.07  A C
ATOM 1551  C   LEU A 228     0.013  44.617  -3.238  1.00 21.13  A C
ATOM 1552  O   LEU A 228    -0.586  45.521  -3.825  1.00 21.22  A O
ATOM 1553  N   GLY A 229     1.222  44.206  -3.591  1.00 20.87  A N
ATOM 1554  CA  GLY A 229     1.891  44.809  -4.723  1.00 21.09  A C
ATOM 1555  C   GLY A 229     1.118  44.480  -5.985  1.00 21.42  A C
ATOM 1556  O   GLY A 229     0.890  45.346  -6.828  1.00 21.71  A O
ATOM 1557  N   ILE A 230     0.710  43.221  -6.120  1.00 21.80  A N
ATOM 1558  CA  ILE A 230    -0.057  42.802  -7.287  1.00 21.79  A C
ATOM 1559  CB  ILE A 230    -0.374  41.299  -7.242  1.00 21.64  A C
ATOM 1560  CG2 ILE A 230    -1.100  40.892  -8.517  1.00 21.38  A C
ATOM 1561  CG1 ILE A 230     0.913  40.488  -7.079  1.00 21.77  A C
ATOM 1562  CD1 ILE A 230     1.813  40.485  -8.302  1.00 22.62  A C
ATOM 1563  C   ILE A 230    -1.383  43.569  -7.315  1.00 22.29  A C
ATOM 1564  O   ILE A 230    -1.819  44.044  -8.367  1.00 21.82  A O
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FIGURE 3A-29

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ATOM 1565  N   LEU A 231   -2.011  43.693  -6.148  1.00 22.88  A N
ATOM 1566  CA  LEU A 231   -3.288  44.390  -6.024  1.00 23.31  A C
ATOM 1567  CB  LEU A 231   -3.790  44.344  -4.573  1.00 23.06  A C
ATOM 1568  CG  LEU A 231   -5.098  45.103  -4.303  1.00 23.69  A C
ATOM 1569  CD1 LEU A 231   -6.236  44.487  -5.102  1.00 23.37  A C
ATOM 1570  CD2 LEU A 231   -5.424  45.069  -2.823  1.00 23.28  A C
ATOM 1571  C   LEU A 231   -3.219  45.841  -6.492  1.00 23.71  A C
ATOM 1572  O   LEU A 231   -4.043  46.266  -7.294  1.00 24.23  A O
ATOM 1573  N   LEU A 232   -2.243  46.600  -5.998  1.00 23.91  A N
ATOM 1574  CA  LEU A 232   -2.121  47.998  -6.394  1.00 23.68  A C
ATOM 1575  CB  LEU A 232   -0.919  48.660  -5.715  1.00 23.78  A C
ATOM 1576  CG  LEU A 232   -1.084  50.132  -5.297  1.00 24.26  A C
ATOM 1577  CD1 LEU A 232    0.279  50.712  -4.987  1.00 23.82  A C
ATOM 1578  CD2 LEU A 232   -1.762  50.949  -6.391  1.00 24.08  A C
ATOM 1579  C   LEU A 232   -1.959  48.091  -7.906  1.00 23.98  A C
ATOM 1580  O   LEU A 232   -2.595  48.925  -8.557  1.00 24.76  A O
ATOM 1581  N   TYR A 233   -1.108  47.235  -8.464  1.00 23.57  A N
ATOM 1582  CA  TYR A 233   -0.874  47.234  -9.903  1.00 23.05  A C
ATOM 1583  CB  TYR A 233    0.209  46.210 -10.276  1.00 21.64  A C
ATOM 1584  CG  TYR A 233    0.533  46.180 -11.756  1.00 20.10  A C
ATOM 1585  CD1 TYR A 233   -0.353  45.619 -12.674  1.00 18.81  A C
ATOM 1586  CE1 TYR A 233   -0.090  45.641 -14.037  1.00 18.22  A C
ATOM 1587  CD2 TYR A 233    1.704  46.762 -12.247  1.00 19.72  A C
ATOM 1588  CE2 TYR A 233    1.978  46.791 -13.616  1.00 18.55  A C
ATOM 1589  CZ  TYR A 233    1.073  46.231 -14.502  1.00 18.85  A C
ATOM 1590  OH  TYR A 233    1.314  46.281 -15.857  1.00 19.45  A O
ATOM 1591  C   TYR A 233   -2.172  46.903 -10.623  1.00 23.64  A C
ATOM 1592  O   TYR A 233   -2.495  47.502 -11.644  1.00 24.49  A O
ATOM 1593  N   ASP A 234   -2.916  45.944 -10.091  1.00 24.15  A N
ATOM 1594  CA  ASP A 234   -4.175  45.561 -10.705  1.00 25.11  A C
ATOM 1595  CB  ASP A 234   -4.845  44.461  -9.888  1.00 25.53  A C
ATOM 1596  CG  ASP A 234   -6.177  44.044 -10.460  1.00 25.90  A C
ATOM 1597  OD1 ASP A 234   -7.123  43.867  -9.670  1.00 27.09  A O
ATOM 1598  OD2 ASP A 234   -6.284  43.886 -11.693  1.00 26.17  A O
ATOM 1599  C   ASP A 234   -5.098  46.773 -10.777  1.00 26.03  A C
ATOM 1600  O   ASP A 234   -5.722  47.029 -11.810  1.00 26.29  A O
ATOM 1601  N   MET A 235   -5.168  47.521  -9.676  1.00 26.30  A N
ATOM 1602  CA  MET A 235   -6.018  48.704  -9.590  1.00 26.73  A C
ATOM 1603  CB  MET A 235   -5.997  49.289  -8.173  1.00 26.52  A C
ATOM 1604  CG  MET A 235   -6.712  48.456  -7.132  1.00 27.65  A C
ATOM 1605  SD  MET A 235   -6.914  49.309  -5.550  1.00 28.52  A S
ATOM 1606  CE  MET A 235   -5.347  49.066  -4.817  1.00 29.19  A C
ATOM 1607  C   MET A 235   -5.661  49.812 -10.568  1.00 27.41  A C
ATOM 1608  O   MET A 235   -6.544  50.365 -11.228  1.00 27.49  A O
ATOM 1609  N   VAL A 236   -4.375  50.137 -10.670  1.00 27.73  A N
ATOM 1610  CA  VAL A 236   -3.955  51.226 -11.546  1.00 27.72  A C
ATOM 1611  CB  VAL A 236   -2.703  51.933 -10.981  1.00 27.14  A C
ATOM 1612  CG1 VAL A 236   -2.978  52.384  -9.558  1.00 27.41  A C
ATOM 1613  CG2 VAL A 236   -1.504  51.007 -11.019  1.00 26.32  A C
ATOM 1614  C   VAL A 236   -3.708  50.860 -13.002  1.00 28.22  A C
ATOM 1615  O   VAL A 236   -3.545  51.746 -13.838  1.00 28.32  A O
ATOM 1616  N   CYS A 237   -3.683  49.568 -13.313  1.00 28.77  A N
ATOM 1617  CA  CYS A 237   -3.468  49.135 -14.693  1.00 29.68  A C
ATOM 1618  CB  CYS A 237   -2.238  48.240 -14.792  1.00 29.71  A C
ATOM 1619  SG  CYS A 237   -0.688  49.093 -14.510  1.00 31.28  A S
ATOM 1620  C   CYS A 237   -4.671  48.389 -15.247  1.00 30.33  A C
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FIGURE 3A-30

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ATOM 1621  O   CYS A 237   -4.797  48.215 -16.460  1.00 30.28  A O
ATOM 1622  N   GLY A 238   -5.550  47.948 -14.351  1.00 30.97  A N
ATOM 1623  CA  GLY A 238   -6.735  47.224 -14.768  1.00 32.39  A C
ATOM 1624  C   GLY A 238   -6.494  45.738 -14.948  1.00 33.64  A C
ATOM 1625  O   GLY A 238   -7.363  45.017 -15.442  1.00 33.64  A O
ATOM 1626  N   ASP A 239   -5.314  45.274 -14.548  1.00 34.84  A N
ATOM 1627  CA  ASP A 239   -4.972  43.863 -14.673  1.00 35.82  A C
ATOM 1628  CB  ASP A 239   -4.681  43.527 -16.134  1.00 37.59  A C
ATOM 1629  CG  ASP A 239   -5.152  42.138 -16.517  1.00 39.57  A C
ATOM 1630  OD1 ASP A 239   -5.046  41.210 -15.679  1.00 40.53  A O
ATOM 1631  OD2 ASP A 239   -5.622  41.974 -17.664  1.00 41.16  A O
ATOM 1632  C   ASP A 239   -3.747  43.515 -13.827  1.00 35.63  A C
ATOM 1633  O   ASP A 239   -3.014  44.397 -13.398  1.00 35.70  A O
ATOM 1634  N   ILE A 240   -3.535  42.224 -13.586  1.00 35.62  A N
ATOM 1635  CA  ILE A 240   -2.389  41.779 -12.808  1.00 35.32  A C
ATOM 1636  CB  ILE A 240   -2.607  40.376 -12.245  1.00 35.08  A C
ATOM 1637  CG2 ILE A 240   -3.702  40.411 -11.199  1.00 34.92  A C
ATOM 1638  CG1 ILE A 240   -2.964  39.415 -13.376  1.00 34.86  A C
ATOM 1639  CD1 ILE A 240   -3.117  37.980 -12.931  1.00 34.38  A C
ATOM 1640  C   ILE A 240   -1.177  41.772 -13.724  1.00 35.52  A C
ATOM 1641  O   ILE A 240   -1.289  41.461 -14.907  1.00 35.69  A O
ATOM 1642  N   PRO A 241    0.002  42.111 -13.183  1.00 35.58  A N
ATOM 1643  CD  PRO A 241    0.196  42.471 -11.768  1.00 35.29  A C
ATOM 1644  CA  PRO A 241    1.274  42.170 -13.913  1.00 35.96  A C
ATOM 1645  CB  PRO A 241    2.194  42.877 -12.925  1.00 35.88  A C
ATOM 1646  CG  PRO A 241    1.695  42.373 -11.609  1.00 35.63  A C
ATOM 1647  C   PRO A 241    1.874  40.858 -14.418  1.00 36.54  A C
ATOM 1648  O   PRO A 241    2.406  40.810 -15.526  1.00 36.27  A O
ATOM 1649  N   PHE A 242    1.794  39.803 -13.611  1.00 37.71  A N
ATOM 1650  CA  PHE A 242    2.353  38.503 -13.982  1.00 38.74  A C
ATOM 1651  CB  PHE A 242    3.301  38.005 -12.884  1.00 36.80  A C
ATOM 1652  CG  PHE A 242    4.204  39.065 -12.327  1.00 35.67  A C
ATOM 1653  CD1 PHE A 242    5.033  39.807 -13.163  1.00 35.12  A C
ATOM 1654  CD2 PHE A 242    4.239  39.313 -10.958  1.00 35.33  A C
ATOM 1655  CE1 PHE A 242    5.887  40.782 -12.643  1.00 35.01  A C
ATOM 1656  CE2 PHE A 242    5.086  40.284 -10.426  1.00 34.83  A C
ATOM 1657  CZ  PHE A 242    5.913  41.020 -11.271  1.00 34.99  A C
ATOM 1658  C   PHE A 242    1.268  37.453 -14.202  1.00 40.46  A C
ATOM 1659  O   PHE A 242    0.274  37.424 -13.478  1.00 40.61  A O
ATOM 1660  N   GLU A 243    1.465  36.589 -15.197  1.00 42.94  A N
ATOM 1661  CA  GLU A 243    0.507  35.522 -15.495  1.00 45.51  A C
ATOM 1662  CB  GLU A 243   -0.114  35.708 -16.892  1.00 47.93  A C
ATOM 1663  CG  GLU A 243    0.902  35.741 -18.043  1.00 52.26  A C
ATOM 1664  CD  GLU A 243    0.271  35.945 -19.430  1.00 54.38  A C
ATOM 1665  OE1 GLU A 243   -0.886  36.421 -19.512  1.00 55.09  A O
ATOM 1666  OE2 GLU A 243    0.948  35.641 -20.444  1.00 55.53  A O
ATOM 1667  C   GLU A 243    1.176  34.149 -15.411  1.00 45.82  A C
ATOM 1668  O   GLU A 243    0.516  33.150 -15.127  1.00 46.16  A O
ATOM 1669  N   HIS A 244    2.486  34.107 -15.648  1.00 45.92  A N
ATOM 1670  CA  HIS A 244    3.237  32.852 -15.605  1.00 46.20  A C
ATOM 1671  CB  HIS A 244    3.907  32.584 -16.956  1.00 46.96  A C
ATOM 1672  CG  HIS A 244    2.982  32.706 -18.124  1.00 48.01  A C
ATOM 1673  CD2 HIS A 244    3.077  33.430 -19.264  1.00 48.07  A C
ATOM 1674  ND1 HIS A 244    1.786  32.024 -18.201  1.00 48.43  A N
ATOM 1675  CE1 HIS A 244    1.183  32.324 -19.338  1.00 48.39  A C
ATOM 1676  NE2 HIS A 244    1.946  33.175 -20.001  1.00 48.59  A N
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FIGURE 3A-31

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ATOM 1677  C   HIS A 244    4.311  32.873 -14.525  1.00 45.97  A C
ATOM 1678  O   HIS A 244    4.801  33.934 -14.141  1.00 46.02  A O
ATOM 1679  N   ASP A 245    4.690  31.691 -14.054  1.00 45.53  A N
ATOM 1680  CA  ASP A 245    5.709  31.580 -13.024  1.00 45.15  A C
ATOM 1681  CB  ASP A 245    5.963  30.109 -12.705  1.00 45.50  A C
ATOM 1682  CG  ASP A 245    4.757  29.439 -12.075  1.00 46.41  A C
ATOM 1683  OD1 ASP A 245    4.844  28.239 -11.739  1.00 47.11  A O
ATOM 1684  OD2 ASP A 245    3.718  30.114 -11.913  1.00 46.66  A O
ATOM 1685  C   ASP A 245    7.013  32.272 -13.409  1.00 44.75  A C
ATOM 1686  O   ASP A 245    7.664  32.877 -12.562  1.00 44.33  A O
ATOM 1687  N   GLU A 246    7.394  32.191 -14.682  1.00 44.79  A N
ATOM 1688  CA  GLU A 246    8.626  32.834 -15.137  1.00 45.23  A C
ATOM 1689  CB  GLU A 246    8.806  32.703 -16.656  1.00 46.50  A C
ATOM 1690  CG  GLU A 246    8.796  31.292 -17.213  1.00 48.66  A C
ATOM 1691  CD  GLU A 246    7.408  30.676 -17.229  1.00 50.00  A C
ATOM 1692  OE1 GLU A 246    6.961  30.178 -16.173  1.00 50.50  A O
ATOM 1693  OE2 GLU A 246    6.758  30.701 -18.300  1.00 50.89  A O
ATOM 1694  C   GLU A 246    8.575  34.318 -14.790  1.00 44.45  A C
ATOM 1695  O   GLU A 246    9.495  34.855 -14.176  1.00 44.55  A O
ATOM 1696  N   GLU A 247    7.493  34.975 -15.198  1.00 43.56  A N
ATOM 1697  CA  GLU A 247    7.313  36.400 -14.942  1.00 42.74  A C
ATOM 1698  CB  GLU A 247    5.947  36.861 -15.444  1.00 43.13  A C
ATOM 1699  CG  GLU A 247    5.760  36.822 -16.946  1.00 43.62  A C
ATOM 1700  CD  GLU A 247    4.313  37.057 -17.336  1.00 44.52  A C
ATOM 1701  OE1 GLU A 247    3.470  36.195 -17.021  1.00 45.06  A O
ATOM 1702  OE2 GLU A 247    4.009  38.103 -17.942  1.00 45.42  A O
ATOM 1703  C   GLU A 247    7.431  36.724 -13.458  1.00 41.88  A C
ATOM 1704  O   GLU A 247    8.057  37.714 -13.083  1.00 42.05  A O
ATOM 1705  N   ILE A 248    6.827  35.891 -12.616  1.00 40.84  A N
ATOM 1706  CA  ILE A 248    6.871  36.107 -11.176  1.00 39.99  A C
ATOM 1707  CB  ILE A 248    5.967  35.097 -10.433  1.00 39.47  A C
ATOM 1708  CG2 ILE A 248    6.034  35.332  -8.932  1.00 38.57  A C
ATOM 1709  CG1 ILE A 248    4.523  35.254 -10.913  1.00 39.17  A C
ATOM 1710  CD1 ILE A 248    3.546  34.324 -10.236  1.00 39.05  A C
ATOM 1711  C   ILE A 248    8.291  36.031 -10.610  1.00 40.10  A C
ATOM 1712  O   ILE A 248    8.722  36.935  -9.886  1.00 39.68  A O
ATOM 1713  N   ILE A 249    9.026  34.968 -10.935  1.00 40.15  A N
ATOM 1714  CA  ILE A 249   10.387  34.839 -10.420  1.00 40.03  A C
ATOM 1715  CB  ILE A 249   10.987  33.427 -10.664  1.00 39.75  A C
ATOM 1716  CG2 ILE A 249   10.123  32.374  -9.995  1.00 39.56  A C
ATOM 1717  CG1 ILE A 249   11.111  33.153 -12.159  1.00 40.35  A C
ATOM 1718  CD1 ILE A 249   11.758  31.819 -12.476  1.00 41.06  A C
ATOM 1719  C   ILE A 249   11.318  35.883 -11.028  1.00 39.63  A C
ATOM 1720  O   ILE A 249   12.336  36.229 -10.429  1.00 39.81  A O
ATOM 1721  N   ARG A 250   10.975  36.391 -12.208  1.00 39.10  A N
ATOM 1722  CA  ARG A 250   11.817  37.405 -12.835  1.00 39.09  A C
ATOM 1723  CB  ARG A 250   11.562  37.483 -14.341  1.00 38.30  A C
ATOM 1724  CG  ARG A 250   12.608  38.315 -15.063  1.00 37.35  A C
ATOM 1725  CD  ARG A 250   12.199  38.645 -16.482  1.00 37.19  A C
ATOM 1726  NE  ARG A 250   13.108  39.620 -17.075  1.00 36.66  A N
ATOM 1727  CZ  ARG A 250   12.778  40.459 -18.052  1.00 36.72  A C
ATOM 1728  NH1 ARG A 250   11.552  40.448 -18.557  1.00 36.16  A N
ATOM 1729  NH2 ARG A 250   13.673  41.318 -18.519  1.00 36.93  A N
ATOM 1730  C   ARG A 250   11.529  38.757 -12.188  1.00 39.36  A C
ATOM 1731  O   ARG A 250   12.401  39.625 -12.116  1.00 39.77  A O
ATOM 1732  N   GLY A 251   10.291  38.925 -11.728  1.00 39.34  A N
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FIGURE 3A-32

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ATOM 1733  CA  GLY A 251     9.887  40.150 -11.063  1.00 39.16  A C
ATOM 1734  C   GLY A 251    10.027  41.455 -11.823  1.00 39.12  A C
ATOM 1735  O   GLY A 251    10.113  42.515 -11.207  1.00 39.50  A O
ATOM 1736  N   GLN A 252    10.047  41.396 -13.151  1.00 38.91  A N
ATOM 1737  CA  GLN A 252    10.162  42.610 -13.958  1.00 38.40  A C
ATOM 1738  CB  GLN A 252    10.737  42.289 -15.335  1.00 39.40  A C
ATOM 1739  CG  GLN A 252    11.178  43.516 -16.107  1.00 40.02  A C
ATOM 1740  CD  GLN A 252    12.538  44.010 -15.661  1.00 40.80  A C
ATOM 1741  OE1 GLN A 252    12.954  45.118 -16.008  1.00 41.78  A O
ATOM 1742  NE2 GLN A 252    13.247  43.184 -14.896  1.00 40.12  A N
ATOM 1743  C   GLN A 252     8.772  43.199 -14.138  1.00 37.66  A C
ATOM 1744  O   GLN A 252     7.881  42.537 -14.673  1.00 37.99  A O
ATOM 1745  N   VAL A 253     8.578  44.438 -13.704  1.00 36.59  A N
ATOM 1746  CA  VAL A 253     7.264  45.056 -13.831  1.00 35.43  A C
ATOM 1747  CB  VAL A 253     6.855  45.778 -12.524  1.00 34.84  A C
ATOM 1748  CG1 VAL A 253     5.449  46.332 -12.648  1.00 33.84  A C
ATOM 1749  CG2 VAL A 253     6.933  44.815 -11.356  1.00 34.62  A C
ATOM 1750  C   VAL A 253     7.189  46.046 -14.984  1.00 34.91  A C
ATOM 1751  O   VAL A 253     7.950  47.011 -15.038  1.00 34.86  A O
ATOM 1752  N   PHE A 254     6.270  45.790 -15.910  1.00 34.45  A N
ATOM 1753  CA  PHE A 254     6.062  46.664 -17.059  1.00 34.51  A C
ATOM 1754  CB  PHE A 254     6.179  45.861 -18.363  1.00 35.55  A C
ATOM 1755  CG  PHE A 254     5.645  46.583 -19.580  1.00 37.57  A C
ATOM 1756  CD1 PHE A 254     4.292  46.502 -19.920  1.00 38.13  A C
ATOM 1757  CD2 PHE A 254     6.486  47.364 -20.373  1.00 38.23  A C
ATOM 1758  CE1 PHE A 254     3.787  47.188 -21.030  1.00 38.03  A C
ATOM 1759  CE2 PHE A 254     5.990  48.056 -21.488  1.00 38.39  A C
ATOM 1760  CZ  PHE A 254     4.640  47.966 -21.815  1.00 38.27  A C
ATOM 1761  C   PHE A 254     4.674  47.300 -16.945  1.00 33.90  A C
ATOM 1762  O   PHE A 254     3.715  46.628 -16.577  1.00 34.17  A O
ATOM 1763  N   PHE A 255     4.565  48.592 -17.247  1.00 33.09  A N
ATOM 1764  CA  PHE A 255     3.274  49.272 -17.170  1.00 32.69  A C
ATOM 1765  CB  PHE A 255     3.416  50.615 -16.445  1.00 31.75  A C
ATOM 1766  CG  PHE A 255     3.705  50.475 -14.979  1.00 30.54  A C
ATOM 1767  CD1 PHE A 255     4.994  50.224 -14.531  1.00 29.60  A C
ATOM 1768  CD2 PHE A 255     2.669  50.513 -14.052  1.00 29.71  A C
ATOM 1769  CE1 PHE A 255     5.247  50.007 -13.182  1.00 29.93  A C
ATOM 1770  CE2 PHE A 255     2.911  50.298 -12.705  1.00 29.36  A C
ATOM 1771  CZ  PHE A 255     4.201  50.042 -12.267  1.00 29.80  A C
ATOM 1772  C   PHE A 255     2.630  49.480 -18.534  1.00 33.08  A C
ATOM 1773  O   PHE A 255     3.209  50.103 -19.423  1.00 32.57  A O
ATOM 1774  N   ARG A 256     1.423  48.945 -18.690  1.00 34.14  A N
ATOM 1775  CA  ARG A 256     0.681  49.051 -19.943  1.00 35.28  A C
ATOM 1776  CB  ARG A 256    -0.213  47.821 -20.121  1.00 36.35  A C
ATOM 1777  CG  ARG A 256    -1.326  47.718 -19.083  1.00 38.55  A C
ATOM 1778  CD  ARG A 256    -1.198  46.466 -18.234  1.00 40.30  A C
ATOM 1779  NE  ARG A 256    -1.338  45.248 -19.028  1.00 42.32  A N
ATOM 1780  CZ  ARG A 256    -1.175  44.017 -18.547  1.00 43.34  A C
ATOM 1781  NH1 ARG A 256    -0.864  43.830 -17.270  1.00 43.87  A N
ATOM 1782  NH2 ARG A 256    -1.323  42.970 -19.346  1.00 44.02  A N
ATOM 1783  C   ARG A 256    -0.182  50.311 -19.951  1.00 34.92  A C
ATOM 1784  O   ARG A 256    -0.829  50.632 -20.944  1.00 35.04  A O
ATOM 1785  N   GLN A 257    -0.181  51.018 -18.829  1.00 34.64  A N
ATOM 1786  CA  GLN A 257    -0.963  52.233 -18.676  1.00 34.59  A C
ATOM 1787  CB  GLN A 257    -2.154  51.971 -17.763  1.00 36.06  A C
ATOM 1788  CG  GLN A 257    -3.278  51.188 -18.383  1.00 37.80  A C
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FIGURE 3A-33

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ATOM 1789  CD  GLN A 257    -4.548  52.001 -18.430  1.00 39.27  A C
ATOM 1790  OE1 GLN A 257    -5.642  51.460 -18.600  1.00 40.69  A O
ATOM 1791  NE2 GLN A 257    -4.412  53.318 -18.284  1.00 39.39  A N
ATOM 1792  C   GLN A 257    -0.131  53.346 -18.068  1.00 33.66  A C
ATOM 1793  O   GLN A 257     0.972  53.116 -17.584  1.00 33.66  A O
ATOM 1794  N   ARG A 258    -0.674  54.555 -18.078  1.00 32.84  A N
ATOM 1795  CA  ARG A 258     0.033  55.691 -17.509  1.00 31.69  A C
ATOM 1796  CB  ARG A 258    -0.524  56.999 -18.075  1.00 31.07  A C
ATOM 1797  CG  ARG A 258     0.427  58.169 -17.966  1.00 31.14  A C
ATOM 1798  CD  ARG A 258     0.606  58.630 -16.540  1.00 32.07  A C
ATOM 1799  NE  ARG A 258     1.773  59.496 -16.425  1.00 33.54  A N
ATOM 1800  CZ  ARG A 258     2.046  60.262 -15.372  1.00 34.00  A C
ATOM 1801  NH1 ARG A 258     1.228  60.281 -14.326  1.00 34.22  A N
ATOM 1802  NH2 ARG A 258     3.145  61.006 -15.364  1.00 33.81  A N
ATOM 1803  C   ARG A 258    -0.119  55.674 -15.993  1.00 30.88  A C
ATOM 1804  O   ARG A 258    -1.223  55.800 -15.474  1.00 31.51  A O
ATOM 1805  N   VAL A 259     0.991  55.500 -15.289  1.00 29.87  A N
ATOM 1806  CA  VAL A 259     0.979  55.484 -13.832  1.00 28.83  A C
ATOM 1807  CB  VAL A 259     1.249  54.064 -13.279  1.00 27.94  A C
ATOM 1808  CG1 VAL A 259     1.350  54.100 -11.763  1.00 26.92  A C
ATOM 1809  CG2 VAL A 259     0.135  53.127 -13.697  1.00 26.67  A C
ATOM 1810  C   VAL A 259     2.071  56.430 -13.359  1.00 28.77  A C
ATOM 1811  O   VAL A 259     3.153  56.457 -13.930  1.00 28.78  A O
ATOM 1812  N   SER A 260     1.788  57.209 -12.321  1.00 29.04  A N
ATOM 1813  CA  SER A 260     2.769  58.161 -11.807  1.00 29.30  A C
ATOM 1814  CB  SER A 260     2.174  58.976 -10.655  1.00 28.09  A C
ATOM 1815  OG  SER A 260     1.833  58.152  -9.561  1.00 27.76  A O
ATOM 1816  C   SER A 260     4.055  57.481 -11.354  1.00 30.04  A C
ATOM 1817  O   SER A 260     4.063  56.299 -11.020  1.00 30.23  A O
ATOM 1818  N   PSR A 261     5.143  58.243 -11.353  1.00 31.10  A N
ATOM 1819  CA  PSR A 261     6.448  57.733 -10.956  1.00 31.99  A C
ATOM 1820  CB  PSR A 261     7.497  58.834 -11.079  1.00 33.03  A C
ATOM 1821  OG  PSR A 261     7.564  59.250 -12.427  1.00 36.26  A O
ATOM 1822  C   PSR A 261     6.433  57.205  -9.533  1.00 31.92  A C
ATOM 1823  O   PSR A 261     7.036  56.173  -9.233  1.00 32.44  A O
ATOM 1824  P   PSR A 261     6.915  60.633 -12.882  1.00 38.76  A P
ATOM 1825  O1  PSR A 261     7.686  61.755 -12.306  1.00 38.43  A O
ATOM 1826  O2  PSR A 261     6.949  60.688 -14.414  1.00 38.21  A O
ATOM 1827  O3  PSR A 261     5.404  60.683 -12.500  1.00 37.10  A O
ATOM 1828  N   GLU A 262     5.746  57.919  -8.652  1.00 31.67  A N
ATOM 1829  CA  GLU A 262     5.665  57.507  -7.261  1.00 31.40  A C
ATOM 1830  CB  GLU A 262     5.044  58.620  -6.419  1.00 32.56  A C
ATOM 1831  CG  GLU A 262     6.062  59.635  -5.927  1.00 34.69  A C
ATOM 1832  CD  GLU A 262     5.412  60.870  -5.344  1.00 37.15  A C
ATOM 1833  OE1 GLU A 262     4.358  60.729  -4.685  1.00 38.40  A O
ATOM 1834  OE2 GLU A 262     5.956  61.981  -5.534  1.00 37.97  A O
ATOM 1835  C   GLU A 262     4.883  56.211  -7.097  1.00 30.39  A C
ATOM 1836  O   GLU A 262     5.311  55.317  -6.365  1.00 30.61  A O
ATOM 1837  N   CYS A 263     3.750  56.094  -7.783  1.00 28.93  A N
ATOM 1838  CA  CYS A 263     2.959  54.876  -7.680  1.00 27.70  A C
ATOM 1839  CB  CYS A 263     1.639  55.012  -8.437  1.00 27.39  A C
ATOM 1840  SG  CYS A 263     0.543  53.592  -8.205  1.00 26.70  A S
ATOM 1841  C   CYS A 263     3.769  53.723  -8.252  1.00 27.04  A C
ATOM 1842  O   CYS A 263     3.809  52.632  -7.681  1.00 26.65  A O
ATOM 1843  N   GLN A 264     4.417  53.969  -9.386  1.00 26.34  A N
ATOM 1844  CA  GLN A 264     5.242  52.946 -10.005  1.00 25.65  A C
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FIGURE 3A-34

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ATOM 1845  CB  GLN A 264     5.894  53.472 -11.286  1.00 25.50  A C
ATOM 1846  CG  GLN A 264     5.037  53.308 -12.526  1.00 25.96  A C
ATOM 1847  CD  GLN A 264     5.804  53.558 -13.813  1.00 26.89  A C
ATOM 1848  OE1 GLN A 264     6.957  53.144 -13.955  1.00 26.95  A O
ATOM 1849  NE2 GLN A 264     5.160  54.221 -14.767  1.00 26.68  A N
ATOM 1850  C   GLN A 264     6.317  52.533  -9.012  1.00 25.46  A C
ATOM 1851  O   GLN A 264     6.719  51.370  -8.957  1.00 25.30  A O
ATOM 1852  N   HIS A 265     6.769  53.493  -8.212  1.00 25.49  A N
ATOM 1853  CA  HIS A 265     7.801  53.212  -7.230  1.00 25.46  A C
ATOM 1854  CB  HIS A 265     8.397  54.507  -6.677  1.00 25.94  A C
ATOM 1855  CG  HIS A 265     9.339  54.282  -5.536  1.00 26.84  A C
ATOM 1856  CD2 HIS A 265    10.686  54.149  -5.504  1.00 26.91  A C
ATOM 1857  ND1 HIS A 265     8.903  54.073  -4.244  1.00 27.41  A N
ATOM 1858  CE1 HIS A 265     9.941  53.818  -3.467  1.00 27.22  A C
ATOM 1859  NE2 HIS A 265    11.035  53.857  -4.208  1.00 27.42  A N
ATOM 1860  C   HIS A 265     7.302  52.355  -6.077  1.00 24.83  A C
ATOM 1861  O   HIS A 265     7.976  51.412  -5.672  1.00 24.71  A O
ATOM 1862  N   LEU A 266     6.128  52.686  -5.545  1.00 24.24  A N
ATOM 1863  CA  LEU A 266     5.569  51.923  -4.438  1.00 23.26  A C
ATOM 1864  CB  LEU A 266     4.298  52.587  -3.912  1.00 22.65  A C
ATOM 1865  CG  LEU A 266     3.615  51.860  -2.747  1.00 22.81  A C
ATOM 1866  CD1 LEU A 266     4.581  51.697  -1.581  1.00 21.97  A C
ATOM 1867  CD2 LEU A 266     2.394  52.643  -2.308  1.00 22.48  A C
ATOM 1868  C   LEU A 266     5.263  50.501  -4.887  1.00 23.14  A C
ATOM 1869  O   LEU A 266     5.448  49.550  -4.132  1.00 23.31  A O
ATOM 1870  N   ILE A 267     4.804  50.359  -6.124  1.00 23.22  A N
ATOM 1871  CA  ILE A 267     4.477  49.049  -6.665  1.00 23.41  A C
ATOM 1872  CB  ILE A 267     3.807  49.159  -8.047  1.00 22.37  A C
ATOM 1873  CG2 ILE A 267     3.714  47.780  -8.691  1.00 21.94  A C
ATOM 1874  CG1 ILE A 267     2.425  49.793  -7.905  1.00 21.54  A C
ATOM 1875  CD1 ILE A 267     1.659  49.894  -9.207  1.00 20.68  A C
ATOM 1876  C   ILE A 267     5.703  48.156  -6.801  1.00 24.06  A C
ATOM 1877  O   ILE A 267     5.678  46.992  -6.398  1.00 24.45  A O
ATOM 1878  N   ARG A 268     6.772  48.691  -7.379  1.00 24.72  A N
ATOM 1879  CA  ARG A 268     7.985  47.902  -7.557  1.00 25.19  A C
ATOM 1880  CB  ARG A 268     8.983  48.644  -8.455  1.00 25.28  A C
ATOM 1881  CG  ARG A 268     8.531  48.734  -9.902  1.00 25.54  A C
ATOM 1882  CD  ARG A 268     9.643  49.204 -10.812  1.00 26.16  A C
ATOM 1883  NE  ARG A 268     9.285  49.065 -12.222  1.00 26.81  A N
ATOM 1884  CZ  ARG A 268     8.866  50.063 -12.996  1.00 26.99  A C
ATOM 1885  NH1 ARG A 268     8.756  51.291 -12.500  1.00 27.14  A N
ATOM 1886  NH2 ARG A 268     8.552  49.831 -14.268  1.00 26.09  A N
ATOM 1887  C   ARG A 268     8.623  47.570  -6.218  1.00 25.06  A C
ATOM 1888  O   ARG A 268     9.330  46.569  -6.089  1.00 25.05  A O
ATOM 1889  N   TRP A 269     8.359  48.406  -5.219  1.00 25.01  A N
ATOM 1890  CA  TRP A 269     8.910  48.197  -3.887  1.00 25.45  A C
ATOM 1891  CB  TRP A 269     8.738  49.468  -3.049  1.00 25.08  A C
ATOM 1892  CG  TRP A 269     9.518  49.467  -1.764  1.00 25.17  A C
ATOM 1893  CD2 TRP A 269     9.439  50.437  -0.713  1.00 24.95  A C
ATOM 1894  CE2 TRP A 269    10.352  50.042   0.291  1.00 24.72  A C
ATOM 1895  CE3 TRP A 269     8.686  51.603  -0.521  1.00 25.26  A C
ATOM 1896  CD1 TRP A 269    10.451  48.548  -1.368  1.00 25.27  A C
ATOM 1897  NE1 TRP A 269    10.955  48.887  -0.135  1.00 25.30  A N
ATOM 1898  CZ2 TRP A 269    10.533  50.770   1.468  1.00 24.37  A C
ATOM 1899  CZ3 TRP A 269     8.866  52.326   0.651  1.00 25.57  A C
ATOM 1900  CH2 TRP A 269     9.784  51.904   1.631  1.00 24.90  A C
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FIGURE 3A-35

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ATOM 1901  C   TRP A 269     8.236  47.000  -3.208  1.00 25.87  A C
ATOM 1902  O   TRP A 269     8.906  46.163  -2.601  1.00 26.33  A O
ATOM 1903  N   CYS A 270     6.914  46.921  -3.316  1.00 26.26  A N
ATOM 1904  CA  CYS A 270     6.160  45.814  -2.733  1.00 26.14  A C
ATOM 1905  CB  CYS A 270     4.654  46.072  -2.842  1.00 25.67  A C
ATOM 1906  SG  CYS A 270     4.058  47.478  -1.891  1.00 25.04  A S
ATOM 1907  C   CYS A 270     6.491  44.525  -3.473  1.00 26.43  A C
ATOM 1908  O   CYS A 270     6.431  43.439  -2.902  1.00 27.07  A O
ATOM 1909  N   LEU A 271     6.841  44.652  -4.747  1.00 26.64  A N
ATOM 1910  CA  LEU A 271     7.161  43.493  -5.566  1.00 27.00  A C
ATOM 1911  CB  LEU A 271     6.622  43.693  -6.980  1.00 26.86  A C
ATOM 1912  CG  LEU A 271     5.104  43.815  -7.087  1.00 26.70  A C
ATOM 1913  CD1 LEU A 271     4.706  44.004  -8.544  1.00 26.15  A C
ATOM 1914  CD2 LEU A 271     4.456  42.563  -6.506  1.00 26.92  A C
ATOM 1915  C   LEU A 271     8.643  43.148  -5.639  1.00 27.35  A C
ATOM 1916  O   LEU A 271     9.079  42.492  -6.582  1.00 27.32  A O
ATOM 1917  N   ALA A 272     9.418  43.583  -4.651  1.00 27.97  A N
ATOM 1918  CA  ALA A 272    10.844  43.277  -4.629  1.00 28.63  A C
ATOM 1919  CB  ALA A 272    11.499  43.914  -3.413  1.00 27.60  A C
ATOM 1920  C   ALA A 272    11.020  41.760  -4.584  1.00 29.58  A C
ATOM 1921  O   ALA A 272    10.279  41.067  -3.886  1.00 29.68  A O
ATOM 1922  N   LEU A 273    11.996  41.247  -5.332  1.00 30.65  A N
ATOM 1923  CA  LEU A 273    12.258  39.810  -5.368  1.00 31.47  A C
ATOM 1924  CB  LEU A 273    13.369  39.495  -6.373  1.00 31.72  A C
ATOM 1925  CG  LEU A 273    12.988  39.533  -7.854  1.00 32.25  A C
ATOM 1926  CD1 LEU A 273    12.004  38.420  -8.158  1.00 32.17  A C
ATOM 1927  CD2 LEU A 273    12.379  40.885  -8.196  1.00 33.84  A C
ATOM 1928  C   LEU A 273    12.639  39.271  -3.994  1.00 32.04  A C
ATOM 1929  O   LEU A 273    12.154  38.218  -3.579  1.00 32.27  A O
ATOM 1930  N   ARG A 274    13.508  39.992  -3.290  1.00 32.68  A N
ATOM 1931  CA  ARG A 274    13.933  39.577  -1.958  1.00 33.87  A C
ATOM 1932  CB  ARG A 274    15.298  40.184  -1.609  1.00 35.70  A C
ATOM 1933  CG  ARG A 274    15.995  39.491  -0.440  1.00 38.98  A C
ATOM 1934  CD  ARG A 274    17.102  40.348   0.173  1.00 41.92  A C
ATOM 1935  NE  ARG A 274    17.961  40.955  -0.840  1.00 45.22  A N
ATOM 1936  CZ  ARG A 274    18.704  40.276  -1.711  1.00 46.69  A C
ATOM 1937  NH1 ARG A 274    18.705  38.945  -1.701  1.00 47.07  A N
ATOM 1938  NH2 ARG A 274    19.442  40.934  -2.602  1.00 47.11  A N
ATOM 1939  C   ARG A 274    12.898  40.041  -0.933  1.00 33.36  A C
ATOM 1940  O   ARG A 274    12.675  41.238  -0.758  1.00 33.73  A O
ATOM 1941  N   PRO A 275    12.251  39.094  -0.242  1.00 33.09  A N
ATOM 1942  CD  PRO A 275    12.444  37.639  -0.374  1.00 32.87  A C
ATOM 1943  CA  PRO A 275    11.234  39.394   0.770  1.00 32.97  A C
ATOM 1944  CB  PRO A 275    11.046  38.050   1.465  1.00 32.82  A C
ATOM 1945  CG  PRO A 275    11.232  37.084   0.346  1.00 32.81  A C
ATOM 1946  C   PRO A 275    11.611  40.507   1.754  1.00 33.33  A C
ATOM 1947  O   PRO A 275    10.819  41.418   2.004  1.00 33.43  A O
ATOM 1948  N   SER A 276    12.819  40.433   2.310  1.00 33.50  A N
ATOM 1949  CA  SER A 276    13.277  41.433   3.272  1.00 33.47  A C
ATOM 1950  CB  SER A 276    14.606  41.003   3.906  1.00 33.83  A C
ATOM 1951  OG  SER A 276    15.670  41.033   2.968  1.00 34.30  A O
ATOM 1952  C   SER A 276    13.434  42.816   2.648  1.00 33.37  A C
ATOM 1953  O   SER A 276    13.561  43.813   3.362  1.00 33.64  A O
ATOM 1954  N   ASP A 277    13.428  42.875   1.318  1.00 33.25  A N
ATOM 1955  CA  ASP A 277    13.562  44.146   0.607  1.00 33.06  A C
ATOM 1956  CB  ASP A 277    14.195  43.924  -0.766  1.00 33.66  A C
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FIGURE 3A-36

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ATOM 1957  CG  ASP A 277   15.707  43.880  -0.711  1.00 33.91  A C
ATOM 1958  OD1 ASP A 277   16.324  43.506  -1.729  1.00 34.61  A O
ATOM 1959  OD2 ASP A 277   16.279  44.226   0.345  1.00 34.19  A O
ATOM 1960  C   ASP A 277   12.222  44.851   0.435  1.00 32.69  A C
ATOM 1961  O   ASP A 277   12.172  46.021   0.066  1.00 32.73  A O
ATOM 1962  N   ARG A 278   11.136  44.129   0.689  1.00 31.99  A N
ATOM 1963  CA  ARG A 278    9.809  44.709   0.571  1.00 31.22  A C
ATOM 1964  CB  ARG A 278    8.752  43.612   0.538  1.00 30.16  A C
ATOM 1965  CG  ARG A 278    8.815  42.790  -0.716  1.00 28.94  A C
ATOM 1966  CD  ARG A 278    8.087  41.478  -0.582  1.00 28.41  A C
ATOM 1967  NE  ARG A 278    8.545  40.575  -1.628  1.00 28.72  A N
ATOM 1968  CZ  ARG A 278    8.369  39.263  -1.621  1.00 28.26  A C
ATOM 1969  NH1 ARG A 278    7.732  38.680  -0.617  1.00 28.43  A N
ATOM 1970  NH2 ARG A 278    8.852  38.535  -2.614  1.00 28.84  A N
ATOM 1971  C   ARG A 278    9.585  45.606   1.767  1.00 31.37  A C
ATOM 1972  O   ARG A 278   10.251  45.459   2.790  1.00 31.58  A O
ATOM 1973  N   PRO A 279    8.648  46.555   1.652  1.00 31.21  A N
ATOM 1974  CD  PRO A 279    7.925  46.915   0.419  1.00 31.42  A C
ATOM 1975  CA  PRO A 279    8.328  47.492   2.727  1.00 31.29  A C
ATOM 1976  CB  PRO A 279    7.656  48.632   1.984  1.00 31.63  A C
ATOM 1977  CG  PRO A 279    6.895  47.902   0.928  1.00 31.46  A C
ATOM 1978  C   PRO A 279    7.416  46.918   3.798  1.00 31.81  A C
ATOM 1979  O   PRO A 279    6.770  45.886   3.604  1.00 32.40  A O
ATOM 1980  N   THR A 280    7.377  47.601   4.935  1.00 31.99  A N
ATOM 1981  CA  THR A 280    6.518  47.209   6.041  1.00 32.07  A C
ATOM 1982  CB  THR A 280    7.100  47.658   7.393  1.00 32.39  A C
ATOM 1983  OG1 THR A 280    7.248  49.084   7.397  1.00 32.72  A O
ATOM 1984  CG2 THR A 280    8.456  47.022   7.631  1.00 31.97  A C
ATOM 1985  C   THR A 280    5.226  47.974   5.797  1.00 32.00  A C
ATOM 1986  O   THR A 280    5.207  48.924   5.013  1.00 32.18  A O
ATOM 1987  N   PHE A 281    4.148  47.566   6.454  1.00 31.91  A N
ATOM 1988  CA  PHE A 281    2.874  48.251   6.284  1.00 31.72  A C
ATOM 1989  CB  PHE A 281    1.808  47.595   7.161  1.00 32.17  A C
ATOM 1990  CG  PHE A 281    1.382  46.246   6.665  1.00 32.69  A C
ATOM 1991  CD1 PHE A 281    0.625  46.130   5.507  1.00 33.31  A C
ATOM 1992  CD2 PHE A 281    1.781  45.090   7.317  1.00 33.74  A C
ATOM 1993  CE1 PHE A 281    0.276  44.887   5.004  1.00 33.55  A C
ATOM 1994  CE2 PHE A 281    1.437  43.838   6.821  1.00 34.05  A C
ATOM 1995  CZ  PHE A 281    0.684  43.737   5.662  1.00 34.12  A C
ATOM 1996  C   PHE A 281    3.046  49.719   6.636  1.00 31.64  A C
ATOM 1997  O   PHE A 281    2.433  50.595   6.026  1.00 31.49  A O
ATOM 1998  N   GLU A 282    3.908  49.977   7.614  1.00 31.87  A N
ATOM 1999  CA  GLU A 282    4.190  51.338   8.048  1.00 31.78  A C
ATOM 2000  CB  GLU A 282    5.061  51.318   9.305  1.00 32.22  A C
ATOM 2001  CG  GLU A 282    5.660  52.664   9.668  1.00 33.46  A C
ATOM 2002  CD  GLU A 282    6.317  52.660  11.035  1.00 34.27  A C
ATOM 2003  OE1 GLU A 282    7.024  51.680  11.352  1.00 34.15  A O
ATOM 2004  OE2 GLU A 282    6.128  53.642  11.788  1.00 34.77  A O
ATOM 2005  C   GLU A 282    4.891  52.104   6.938  1.00 31.66  A C
ATOM 2006  O   GLU A 282    4.559  53.257   6.668  1.00 31.68  A O
ATOM 2007  N   GLU A 283    5.856  51.456   6.292  1.00 31.63  A N
ATOM 2008  CA  GLU A 283    6.592  52.086   5.206  1.00 32.04  A C
ATOM 2009  CB  GLU A 283    7.780  51.220   4.796  1.00 32.98  A C
ATOM 2010  CG  GLU A 283    8.889  51.211   5.832  1.00 34.14  A C
ATOM 2011  CD  GLU A 283   10.079  50.381   5.413  1.00 34.85  A C
ATOM 2012  OE1 GLU A 283    9.910  49.160   5.200  1.00 34.82  A O
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FIGURE 3A-37

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ATOM 2013  OE2 GLU A 283    11.185  50.953   5.300  1.00 35.88  A O
ATOM 2014  C   GLU A 283     5.710  52.369   3.996  1.00 32.13  A C
ATOM 2015  O   GLU A 283     5.884  53.385   3.323  1.00 32.62  A O
ATOM 2016  N   ILE A 284     4.762  51.479   3.717  1.00 31.46  A N
ATOM 2017  CA  ILE A 284     3.869  51.686   2.588  1.00 30.84  A C
ATOM 2018  CB  ILE A 284     2.976  50.448   2.333  1.00 30.21  A C
ATOM 2019  CG2 ILE A 284     1.964  50.741   1.235  1.00 29.70  A C
ATOM 2020  CG1 ILE A 284     3.843  49.258   1.917  1.00 29.32  A C
ATOM 2021  CD1 ILE A 284     3.059  47.989   1.656  1.00 27.41  A C
ATOM 2022  C   ILE A 284     2.986  52.907   2.846  1.00 31.23  A C
ATOM 2023  O   ILE A 284     2.917  53.816   2.018  1.00 31.62  A O
ATOM 2024  N   GLN A 285     2.330  52.947   4.002  1.00 30.98  A N
ATOM 2025  CA  GLN A 285     1.453  54.071   4.324  1.00 30.83  A C
ATOM 2026  CB  GLN A 285     0.609  53.744   5.555  1.00 30.48  A C
ATOM 2027  CG  GLN A 285    -0.401  52.639   5.293  1.00 30.38  A C
ATOM 2028  CD  GLN A 285    -1.386  52.463   6.425  1.00 30.29  A C
ATOM 2029  OE1 GLN A 285    -1.051  51.936   7.489  1.00 29.83  A O
ATOM 2030  NE2 GLN A 285    -2.614  52.916   6.205  1.00 30.24  A N
ATOM 2031  C   GLN A 285     2.173  55.402   4.520  1.00 30.98  A C
ATOM 2032  O   GLN A 285     1.551  56.466   4.469  1.00 30.99  A O
ATOM 2033  N   ASN A 286     3.480  55.349   4.748  1.00 31.18  A N
ATOM 2034  CA  ASN A 286     4.255  56.572   4.918  1.00 31.36  A C
ATOM 2035  CB  ASN A 286     5.396  56.357   5.915  1.00 30.79  A C
ATOM 2036  CG  ASN A 286     4.959  56.543   7.356  1.00 30.73  A C
ATOM 2037  OD1 ASN A 286     5.636  56.097   8.279  1.00 31.60  A O
ATOM 2038  ND2 ASN A 286     3.835  57.216   7.557  1.00 30.28  A N
ATOM 2039  C   ASN A 286     4.821  56.981   3.566  1.00 31.43  A C
ATOM 2040  O   ASN A 286     5.481  58.011   3.440  1.00 31.45  A O
ATOM 2041  N   HIS A 287     4.548  56.166   2.553  1.00 31.32  A N
ATOM 2042  CA  HIS A 287     5.035  56.436   1.209  1.00 31.17  A C
ATOM 2043  CB  HIS A 287     4.754  55.240   0.300  1.00 29.93  A C
ATOM 2044  CG  HIS A 287     5.450  55.312  -1.022  1.00 29.31  A C
ATOM 2045  CD2 HIS A 287     6.549  54.671  -1.484  1.00 28.46  A C
ATOM 2046  ND1 HIS A 287     5.042  56.154  -2.033  1.00 29.09  A N
ATOM 2047  CE1 HIS A 287     5.860  56.028  -3.063  1.00 29.04  A C
ATOM 2048  NE2 HIS A 287     6.784  55.135  -2.754  1.00 28.58  A N
ATOM 2049  C   HIS A 287     4.402  57.701   0.625  1.00 31.51  A C
ATOM 2050  O   HIS A 287     3.233  58.002   0.874  1.00 32.07  A O
ATOM 2051  N   PRO A 288     5.177  58.463  -0.156  1.00 31.24  A N
ATOM 2052  CD  PRO A 288     6.610  58.276  -0.439  1.00 30.86  A C
ATOM 2053  CA  PRO A 288     4.689  59.695  -0.770  1.00 31.12  A C
ATOM 2054  CB  PRO A 288     5.828  60.082  -1.697  1.00 30.70  A C
ATOM 2055  CG  PRO A 288     7.019  59.638  -0.924  1.00 30.77  A C
ATOM 2056  C   PRO A 288     3.375  59.535  -1.514  1.00 31.08  A C
ATOM 2057  O   PRO A 288     2.497  60.387  -1.422  1.00 32.24  A O
ATOM 2058  N   TRP A 289     3.233  58.441  -2.247  1.00 30.80  A N
ATOM 2059  CA  TRP A 289     2.017  58.221  -3.016  1.00 30.53  A C
ATOM 2060  CB  TRP A 289     2.215  57.042  -3.973  1.00 29.39  A C
ATOM 2061  CG  TRP A 289     1.058  56.826  -4.892  1.00 27.91  A C
ATOM 2062  CD2 TRP A 289     0.027  55.845  -4.751  1.00 26.99  A C
ATOM 2063  CE2 TRP A 289    -0.884  56.045  -5.809  1.00 27.12  A C
ATOM 2064  CE3 TRP A 289    -0.217  54.817  -3.834  1.00 26.62  A C
ATOM 2065  CD1 TRP A 289     0.743  57.558  -5.998  1.00 27.31  A C
ATOM 2066  NE1 TRP A 289    -0.421  57.097  -6.554  1.00 27.11  A N
ATOM 2067  CZ2 TRP A 289    -2.028  55.255  -5.975  1.00 27.02  A C
ATOM 2068  CZ3 TRP A 289    -1.356  54.027  -3.998  1.00 27.10  A C
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FIGURE 3A-38

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ATOM 2069  CH2 TRP A 289    -2.246  54.253  -5.061  1.00 27.03  A C
ATOM 2070  C   TRP A 289     0.774  57.983  -2.154  1.00 30.97  A C
ATOM 2071  O   TRP A 289    -0.349  58.184  -2.614  1.00 30.43  A O
ATOM 2072  N   MET A 290     0.980  57.570  -0.906  1.00 32.06  A N
ATOM 2073  CA  MET A 290    -0.124  57.279   0.006  1.00 33.53  A C
ATOM 2074  CB  MET A 290     0.293  56.192   1.001  1.00 32.78  A C
ATOM 2075  CG  MET A 290     0.396  54.792   0.410  1.00 32.61  A C
ATOM 2076  SD  MET A 290    -1.205  54.057   0.012  1.00 32.41  A S
ATOM 2077  CE  MET A 290    -1.358  52.861   1.325  1.00 32.97  A C
ATOM 2078  C   MET A 290    -0.670  58.472   0.787  1.00 35.26  A C
ATOM 2079  O   MET A 290    -1.602  58.316   1.582  1.00 36.05  A O
ATOM 2080  N   GLN A 291    -0.112  59.659   0.565  1.00 36.55  A N
ATOM 2081  CA  GLN A 291    -0.566  60.848   1.287  1.00 37.83  A C
ATOM 2082  CB  GLN A 291     0.540  61.910   1.300  1.00 38.93  A C
ATOM 2083  CG  GLN A 291     1.770  61.509   2.106  1.00 41.18  A C
ATOM 2084  CD  GLN A 291     1.406  60.761   3.389  1.00 42.74  A C
ATOM 2085  OE1 GLN A 291     1.202  59.544   3.377  1.00 43.13  A O
ATOM 2086  NE2 GLN A 291     1.308  61.492   4.496  1.00 43.44  A N
ATOM 2087  C   GLN A 291    -1.861  61.468   0.765  1.00 37.92  A C
ATOM 2088  O   GLN A 291    -2.272  61.216  -0.368  1.00 38.01  A O
ATOM 2089  N   ASP A 292    -2.497  62.273   1.614  1.00 37.98  A N
ATOM 2090  CA  ASP A 292    -3.741  62.967   1.277  1.00 38.64  A C
ATOM 2091  CB  ASP A 292    -3.469  64.054   0.238  1.00 40.31  A C
ATOM 2092  CG  ASP A 292    -2.609  65.173   0.782  1.00 42.16  A C
ATOM 2093  OD1 ASP A 292    -2.072  65.951  -0.036  1.00 43.49  A O
ATOM 2094  OD2 ASP A 292    -2.477  65.281   2.026  1.00 43.28  A O
ATOM 2095  C   ASP A 292    -4.857  62.063   0.772  1.00 38.13  A C
ATOM 2096  O   ASP A 292    -5.593  62.426  -0.146  1.00 37.67  A O
ATOM 2097  N   VAL A 293    -4.984  60.891   1.380  1.00 37.74  A N
ATOM 2098  CA  VAL A 293    -6.015  59.948   0.988  1.00 36.92  A C
ATOM 2099  CB  VAL A 293    -5.874  58.620   1.760  1.00 36.63  A C
ATOM 2100  CG1 VAL A 293    -6.085  58.857   3.241  1.00 36.75  A C
ATOM 2101  CG2 VAL A 293    -6.875  57.607   1.240  1.00 36.45  A C
ATOM 2102  C   VAL A 293    -7.380  60.548   1.287  1.00 36.77  A C
ATOM 2103  O   VAL A 293    -7.520  61.363   2.194  1.00 36.28  A O
ATOM 2104  N   LEU A 294    -8.379  60.145   0.510  1.00 37.04  A N
ATOM 2105  CA  LEU A 294    -9.744  60.619   0.693  1.00 36.70  A C
ATOM 2106  CB  LEU A 294   -10.541  60.488  -0.608  1.00 36.31  A C
ATOM 2107  CG  LEU A 294   -10.184  61.373  -1.797  1.00 35.98  A C
ATOM 2108  CD1 LEU A 294   -11.121  61.055  -2.958  1.00 35.56  A C
ATOM 2109  CD2 LEU A 294   -10.299  62.833  -1.399  1.00 35.35  A C
ATOM 2110  C   LEU A 294   -10.431  59.774   1.753  1.00 36.93  A C
ATOM 2111  O   LEU A 294    -9.994  58.662   2.050  1.00 36.89  A O
ATOM 2112  N   LEU A 295   -11.511  60.308   2.317  1.00 37.27  A N
ATOM 2113  CA  LEU A 295   -12.285  59.591   3.320  1.00 37.34  A C
ATOM 2114  CB  LEU A 295   -13.111  60.571   4.150  1.00 37.61  A C
ATOM 2115  CG  LEU A 295   -12.317  61.616   4.938  1.00 38.05  A C
ATOM 2116  CD1 LEU A 295   -13.267  62.655   5.514  1.00 37.84  A C
ATOM 2117  CD2 LEU A 295   -11.525  60.933   6.044  1.00 37.79  A C
ATOM 2118  C   LEU A 295   -13.207  58.655   2.552  1.00 37.69  A C
ATOM 2119  O   LEU A 295   -13.495  58.883   1.377  1.00 37.67  A O
ATOM 2120  N   PRO A 296   -13.674  57.580   3.195  1.00 38.07  A N
ATOM 2121  CD  PRO A 296   -13.305  57.036   4.513  1.00 37.73  A C
ATOM 2122  CA  PRO A 296   -14.561  56.663   2.477  1.00 38.61  A C
ATOM 2123  CB  PRO A 296   -14.935  55.649   3.551  1.00 38.60  A C
ATOM 2124  CG  PRO A 296   -13.664  55.576   4.362  1.00 38.08  A C
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FIGURE 3A-39

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ATOM 2125  C   PRO A 296  -15.776  57.346   1.846  1.00 39.37  A C
ATOM 2126  O   PRO A 296  -16.075  57.124   0.672  1.00 39.15  A O
ATOM 2127  N   GLN A 297  -16.466  58.185   2.615  1.00 40.53  A N
ATOM 2128  CA  GLN A 297  -17.643  58.882   2.097  1.00 41.54  A C
ATOM 2129  CB  GLN A 297  -18.342  59.683   3.201  1.00 42.00  A C
ATOM 2130  CG  GLN A 297  -19.703  60.226   2.776  1.00 43.00  A C
ATOM 2131  CD  GLN A 297  -20.612  59.145   2.202  1.00 44.13  A C
ATOM 2132  OE1 GLN A 297  -21.048  58.235   2.910  1.00 44.03  A O
ATOM 2133  NE2 GLN A 297  -20.891  59.238   0.905  1.00 45.11  A N
ATOM 2134  C   GLN A 297  -17.277  59.806   0.942  1.00 41.76  A C
ATOM 2135  O   GLN A 297  -17.993  59.866  -0.056  1.00 42.14  A O
ATOM 2136  N   GLU A 298  -16.174  60.534   1.077  1.00 41.95  A N
ATOM 2137  CA  GLU A 298  -15.733  61.416   0.004  1.00 42.55  A C
ATOM 2138  CB  GLU A 298  -14.416  62.108   0.371  1.00 42.98  A C
ATOM 2139  CG  GLU A 298  -14.534  63.222   1.387  1.00 44.14  A C
ATOM 2140  CD  GLU A 298  -13.179  63.772   1.799  1.00 45.20  A C
ATOM 2141  OE1 GLU A 298  -13.142  64.794   2.520  1.00 46.25  A O
ATOM 2142  OE2 GLU A 298  -12.150  63.179   1.407  1.00 44.80  A O
ATOM 2143  C   GLU A 298  -15.513  60.566  -1.245  1.00 42.63  A C
ATOM 2144  O   GLU A 298  -15.956  60.915  -2.337  1.00 42.92  A O
ATOM 2145  N   THR A 299  -14.825  59.442  -1.066  1.00 42.59  A N
ATOM 2146  CA  THR A 299  -14.528  58.537  -2.167  1.00 42.62  A C
ATOM 2147  CB  THR A 299  -13.803  57.271  -1.669  1.00 42.32  A C
ATOM 2148  OG1 THR A 299  -12.682  57.648  -0.861  1.00 42.76  A O
ATOM 2149  CG2 THR A 299  -13.314  56.443  -2.843  1.00 41.47  A C
ATOM 2150  C   THR A 299  -15.809  58.117  -2.874  1.00 42.61  A C
ATOM 2151  O   THR A 299  -15.851  58.026  -4.099  1.00 42.88  A O
ATOM 2152  N   ALA A 300  -16.853  57.864  -2.096  1.00 42.68  A N
ATOM 2153  CA  ALA A 300  -18.130  57.447  -2.657  1.00 42.89  A C
ATOM 2154  CB  ALA A 300  -19.081  57.034  -1.542  1.00 42.68  A C
ATOM 2155  C   ALA A 300  -18.750  58.561  -3.483  1.00 43.19  A C
ATOM 2156  O   ALA A 300  -19.160  58.343  -4.620  1.00 43.47  A O
ATOM 2157  N   GLU A 301  -18.809  59.756  -2.905  1.00 43.41  A N
ATOM 2158  CA  GLU A 301  -19.391  60.914  -3.574  1.00 43.84  A C
ATOM 2159  CB  GLU A 301  -19.358  62.132  -2.648  1.00 44.85  A C
ATOM 2160  CG  GLU A 301  -20.431  62.139  -1.572  1.00 46.58  A C
ATOM 2161  CD  GLU A 301  -20.252  63.276  -0.574  1.00 48.06  A C
ATOM 2162  OE1 GLU A 301  -21.177  63.496   0.240  1.00 49.05  A O
ATOM 2163  OE2 GLU A 301  -19.190  63.943  -0.597  1.00 48.02  A O
ATOM 2164  C   GLU A 301  -18.710  61.278  -4.883  1.00 43.56  A C
ATOM 2165  O   GLU A 301  -19.373  61.628  -5.858  1.00 43.87  A O
ATOM 2166  N   ILE A 302  -17.387  61.192  -4.901  1.00 43.12  A N
ATOM 2167  CA  ILE A 302  -16.618  61.543  -6.085  1.00 42.30  A C
ATOM 2168  CB  ILE A 302  -15.182  61.936  -5.707  1.00 41.90  A C
ATOM 2169  CG2 ILE A 302  -14.424  62.396  -6.939  1.00 41.79  A C
ATOM 2170  CG1 ILE A 302  -15.200  63.049  -4.667  1.00 41.67  A C
ATOM 2171  CD1 ILE A 302  -13.820  63.453  -4.198  1.00 41.60  A C
ATOM 2172  C   ILE A 302  -16.522  60.453  -7.143  1.00 42.44  A C
ATOM 2173  O   ILE A 302  -16.597  60.740  -8.336  1.00 42.27  A O
ATOM 2174  N   HIS A 303  -16.363  59.205  -6.711  1.00 42.56  A N
ATOM 2175  CA  HIS A 303  -16.189  58.097  -7.649  1.00 42.80  A C
ATOM 2176  CB  HIS A 303  -14.837  57.424  -7.384  1.00 41.08  A C
ATOM 2177  CG  HIS A 303  -13.665  58.349  -7.487  1.00 39.57  A C
ATOM 2178  CD2 HIS A 303  -12.898  58.924  -6.531  1.00 38.64  A C
ATOM 2179  ND1 HIS A 303  -13.161  58.782  -8.694  1.00 38.96  A N
ATOM 2180  CE1 HIS A 303  -12.132  59.583  -8.477  1.00 38.56  A C
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FIGURE 3A-40

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ATOM 2181  NE2 HIS A 303  -11.953  59.686  -7.173  1.00 38.04  A N
ATOM 2182  C   HIS A 303  -17.259  57.009  -7.690  1.00 44.03  A C
ATOM 2183  O   HIS A 303  -17.271  56.199  -8.615  1.00 43.91  A O
ATOM 2184  N   LEU A 304  -18.157  56.975  -6.714  1.00 45.62  A N
ATOM 2185  CA  LEU A 304  -19.160  55.918  -6.701  1.00 47.23  A C
ATOM 2186  CB  LEU A 304  -19.076  55.177  -5.369  1.00 46.59  A C
ATOM 2187  CG  LEU A 304  -17.652  54.716  -5.045  1.00 45.72  A C
ATOM 2188  CD1 LEU A 304  -17.633  53.993  -3.712  1.00 45.64  A C
ATOM 2189  CD2 LEU A 304  -17.140  53.814  -6.156  1.00 45.10  A C
ATOM 2190  C   LEU A 304  -20.607  56.318  -6.994  1.00 48.86  A C
ATOM 2191  O   LEU A 304  -21.342  55.561  -7.628  1.00 48.95  A O
ATOM 2192  N   HIS A 305  -21.023  57.495  -6.538  1.00 50.81  A N
ATOM 2193  CA  HIS A 305  -22.391  57.948  -6.781  1.00 52.83  A C
ATOM 2194  CB  HIS A 305  -22.759  59.084  -5.817  1.00 53.66  A C
ATOM 2195  CG  HIS A 305  -22.748  58.683  -4.372  1.00 54.94  A C
ATOM 2196  CD2 HIS A 305  -22.613  57.469  -3.784  1.00 55.00  A C
ATOM 2197  ND1 HIS A 305  -22.881  59.593  -3.345  1.00 55.12  A N
ATOM 2198  CE1 HIS A 305  -22.825  58.960  -2.187  1.00 55.26  A C
ATOM 2199  NE2 HIS A 305  -22.663  57.670  -2.425  1.00 55.25  A N
ATOM 2200  C   HIS A 305  -22.543  58.423  -8.226  1.00 53.63  A C
ATOM 2201  O   HIS A 305  -23.322  57.790  -8.977  1.00 53.81  A O
ATOM 2202  OXT HIS A 305  -21.874  59.418  -8.591  1.00 54.41  A O
TER        1   HIS A 305                                      A
HET  2203  O   HOH W   1    5.028  44.768   8.332  1.00 30.17  W O
HET  2204  O   HOH W   2    8.189  38.473   7.347  1.00 29.96  W O
HET  2205  O   HOH W   3  -15.166  38.011   6.469  1.00 38.94  W O
HET  2206  O   HOH W   4   -2.980  38.949   5.561  1.00 14.04  W O
HET  2207  O   HOH W   5    5.819  34.261   9.032  1.00 32.20  W O
HET  2208  O   HOH W   6    2.651  36.873  -7.927  1.00 21.87  W O
HET  2209  O   HOH W   7   -8.247  33.214   2.755  1.00 16.11  W O
HET  2210  O   HOH W   8  -17.539  45.069   9.101  1.00 42.43  W O
HET  2211  O   HOH W   9    0.205  38.625 -11.274  1.00 27.72  W O
HET  2212  O   HOH W  10    8.601  39.365 -15.205  1.00 19.93  W O
HET  2213  O   HOH W  12  -12.178  27.032   6.042  1.00 34.29  W O
HET  2214  O   HOH W  13  -14.652  33.066   5.890  1.00 28.78  W O
HET  2215  O   HOH W  14    5.504  37.244   9.057  1.00 48.44  W O
HET  2216  O   HOH W  15  -10.014  53.379 -17.265  1.00 41.36  W O
HET  2217  O   HOH W  16  -11.733  55.657 -11.556  1.00 31.86  W O
HET  2218  O   HOH W  18   -9.067  42.492 -13.410  1.00 31.57  W O
HET  2219  O   HOH W  19   -3.301  54.461  10.306  1.00 29.67  W O
HET  2220  O   HOH W  20    4.634  47.588   9.605  1.00 26.06  W O
HET  2221  O   HOH W  21  -15.737  35.886   4.408  1.00 30.22  W O
HET  2222  O   HOH W  22    1.740  48.969  10.693  1.00 17.77  W O
HET  2223  O   HOH W  23   -2.124  37.491   0.591  1.00 18.68  W O
HET  2224  O   HOH W  24   -7.503  59.204  -2.056  1.00 24.14  W O
HET  2225  O   HOH W  25   14.691  42.500  -3.819  1.00 27.42  W O
HET  2226  O   HOH W  26   -5.015  58.805 -12.772  1.00 37.56  W O
HET  2227  O   HOH W  27  -12.893  49.920   5.111  1.00 27.25  W O
HET  2228  O   HOH W  28  -10.526  49.970   6.159  1.00 30.61  W O
HET  2229  O   HOH W  29  -10.579  55.841   1.956  1.00 37.09  W O
HET  2230  O   HOH W  30    8.174  55.239   3.025  1.00 35.98  W O
HET  2231  O   HOH W  31   -4.703  54.860 -13.350  1.00 34.79  W O
HET  2232  O   HOH W  33   -2.521  59.537   3.727  1.00 32.97  W O
HET  2233  O   HOH W  34   -6.902  39.184 -10.274  1.00 37.92  W O
HET  2234  O   HOH W  35  -25.018  22.780   4.471  1.00 38.82  W O
HET  2235  O   HOH W  37   11.110  45.626  -8.454  1.00 63.51  W O
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FIGURE 3A-41

HET	2236	O	HOH	W	38	3.233	26.257	7.352	1.00	49.82	W	O
HET	2237	O	HOH	W	39	-8.993	46.605	-16.788	1.00	36.24	W	O
HET	2238	O	HOH	W	40	-4.624	36.022	-3.347	1.00	30.42	W	O
HET	2239	O	HOH	W	42	-8.156	51.431	10.620	1.00	53.74	W	O
HET	2240	O	HOH	W	44	8.873	50.024	9.599	1.00	26.09	W	O
HET	2241	O	HOH	W	46	15.002	39.397	-12.496	1.00	50.24	W	O
HET	2242	O	HOH	W	48	9.190	23.988	1.721	1.00	38.24	W	O
HET	2243	O	HOH	W	49	-29.966	30.019	-6.829	1.00	46.18	W	O
HET	2244	O	HOH	W	50	-8.357	50.437	-18.165	1.00	28.28	W	O
HET	2245	O	HOH	W	51	-31.637	29.667	-3.497	1.00	37.94	W	O
HET	2246	O	HOH	W	52	-0.812	35.480	-0.610	1.00	24.16	W	O
HET	2247	O	HOH	W	55	7.743	65.356	-13.441	1.00	51.25	W	O
HET	2248	O	HOH	W	56	-19.349	16.749	3.307	1.00	58.24	W	O
HET	2249	O	HOH	W	59	-25.068	57.066	8.935	1.00	43.95	W	O
HET	2250	O	HOH	W	60	-6.064	61.348	-2.514	1.00	30.32	W	O
HET	2251	O	HOH	W	61	-2.366	34.318	16.286	1.00	40.09	W	O
HET	2252	O	HOH	W	63	10.473	43.256	-8.863	1.00	33.73	W	O
HET	2253	O	HOH	W	64	-1.891	37.597	3.438	1.00	27.48	W	O
HET	2254	O	HOH	W	65	8.073	35.702	2.455	1.00	42.54	W	O
HET	2255	O	HOH	W	67	-7.043	63.544	-4.235	1.00	41.47	W	O
HET	2256	O	HOH	W	69	1.372	36.509	-1.864	1.00	26.24	W	O
HET	2257	O	HOH	W	71	-18.454	24.863	-4.559	1.00	62.61	W	O
HET	2258	O	HOH	W	72	-19.939	24.139	-2.665	1.00	44.21	W	O
HET	2259	O	HOH	W	74	-0.878	62.275	-3.204	1.00	31.73	W	O
HET	2260	O	HOH	W	76	9.361	61.465	-14.860	1.00	39.25	W	O
HET	2261	O	HOH	W	77	-13.726	57.212	-10.884	1.00	35.78	W	O
HET	2262	O	HOH	W	78	10.067	52.729	-10.435	1.00	35.42	W	O
HET	2263	O	HOH	W	79	7.053	43.341	4.431	1.00	23.74	W	O
HET	2264	O	HOH	W	80	-15.738	58.872	6.089	1.00	50.27	W	O
HET	2265	O	HOH	W	83	-11.985	33.169	-3.657	1.00	48.41	W	O
HET	2266	O	HOH	W	84	-17.971	23.353	-0.678	1.00	52.72	W	O
HET	2267	O	HOH	W	85	1.104	51.366	9.124	1.00	19.42	W	O
HET	2268	O	HOH	W	86	0.430	27.592	-5.525	1.00	26.70	W	O
HET	2269	O	HOH	W	87	0.645	36.162	3.793	1.00	31.58	W	O
HET	2270	O	HOH	W	88	10.165	38.535	5.436	1.00	44.92	W	O
HET	2271	O	HOH	W	89	12.085	47.218	4.404	1.00	34.05	W	O
HET	2272	O	HOH	W	90	-5.602	49.658	10.949	1.00	31.77	W	O
HET	2273	O	HOH	W	91	0.406	34.678	1.571	1.00	47.69	W	O
HET	2274	O	HOH	W	92	-23.782	29.350	-10.256	1.00	42.70	W	O
HET	2275	O	HOH	W	93	-19.758	41.777	-7.221	1.00	28.35	W	O
HET	2276	O	HOH	W	94	6.066	32.502	15.452	1.00	50.39	W	O
HET	2277	O	HOH	W	96	9.202	39.065	-17.522	1.00	25.41	W	O
HET	2278	O	HOH	W	97	-19.149	31.406	-9.369	1.00	35.00	W	O
HET	2279	O	HOH	W	99	-3.415	29.086	2.112	1.00	44.42	W	O
HET	2280	O	HOH	W	100	-11.244	32.868	17.778	1.00	46.43	W	O
HET	2281	O	HOH	W	101	-6.371	60.625	-9.318	1.00	20.35	W	O
HET	2282	O	HOH	W	102	-14.821	49.463	6.812	1.00	50.68	W	O
HET	2283	O	HOH	W	103	-20.628	43.673	-10.854	1.00	39.24	W	O
HET	2284	O	HOH	W	104	-3.499	32.121	-10.335	1.00	46.91	W	O
HET	2285	O	HOH	W	105	-4.206	30.482	-8.410	1.00	41.69	W	O
HET	2286	O	HOH	W	106	-2.517	34.615	-2.667	1.00	48.27	W	O
HET	2287	O	HOH	W	107	-19.491	49.493	5.239	1.00	54.59	W	O
HET	2288	O	HOH	W	108	11.670	23.954	3.270	1.00	59.77	W	O
HET	2289	O	HOH	W	110	10.956	50.968	-5.659	1.00	37.53	W	O
HET	2290	O	HOH	W	112	-4.243	62.123	-7.733	1.00	31.89	W	O
HET	2291	O	HOH	W	113	2.869	29.235	-14.985	1.00	58.33	W	O

FIGURE 3A-42

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HET  2292  O   HOH W 114     4.970  56.477  11.644  1.00 37.38  W O
HET  2293  O   HOH W 115    -2.277  27.663  -5.123  1.00 53.27  W O
HET  2294  O   HOH W 116   -25.920  44.829  -3.971  1.00 39.10  W O
HET  2295  O   HOH W 117    -2.918  28.265  10.863  1.00 34.48  W O
HET  2296  O   HOH W 118     1.093  31.480  16.111  1.00 38.19  W O
HET  2297  O   HOH W 119   -22.414  42.136  -7.347  1.00 46.41  W O
HET  2298  O   HOH W 120     4.651  43.405 -15.563  1.00 30.39  W O
HET  2299  O   HOH W 121   -10.047  32.408  -0.635  1.00 45.93  W O
HET  2300  O   HOH W 122   -19.404  36.073  -8.436  1.00 52.65  W O
HET  2301  O   HOH W 124   -15.398  22.505  -4.803  1.00 41.66  W O
HET  2302  O   HOH W 125   -25.154  42.786   7.198  1.00 35.04  W O
HET  2303  O   HOH W 126     9.795  42.939   4.202  1.00 41.67  W O
HET  2304  O   HOH W 127    10.504  46.370 -12.440  1.00 45.18  W O
HET  2305  O   HOH W 128   -16.449  49.115   8.910  1.00 32.05  W O
HET  2306  O   HOH W 129   -28.785  28.143   2.251  1.00 50.49  W O
HET  2307  O   HOH W 130     9.581  56.962 -13.351  1.00 36.93  W O
HET  2308  O   HOH W 131     0.326  23.925   0.259  1.00 42.39  W O
HET  2309  O   HOH W 132   -31.287  42.433   0.878  1.00 42.32  W O
HET  2310  O   HOH W 133   -25.630  42.964  -0.961  1.00 42.68  W O
HET  2311  O   HOH W 134   -10.529  48.443   9.728  1.00 27.22  W O
HET  2312  O   HOH W 135    13.634  43.596  -6.888  1.00 48.18  W O
HET  2313  O   HOH W 136   -21.363  29.135  -9.356  1.00 30.28  W O
HET  2314  O   HOH W 137     5.433  29.626  15.277  1.00 46.55  W O
HET  2315  O   HOH W 138   -21.620  32.893 -10.535  1.00 47.34  W O
HET  2316  O   HOH W 140     1.071  27.588  10.155  1.00 40.25  W O
HET  2317  O   HOH W 141    13.495  30.308   3.209  1.00 43.20  W O
HET  2318  O   HOH W 142   -21.940  38.568  -7.406  1.00 56.63  W O
HET  2319  O   HOH W 143    -0.195  29.774  10.882  1.00 45.91  W O
HET  2320  O   HOH W 144   -11.723  29.261  -5.968  1.00 52.48  W O
HET  2321  O   HOH W 145    11.930  51.561  -8.676  1.00 44.58  W O
HET  2322  O   HOH W 146   -22.617  58.131   9.053  1.00 39.70  W O
HET  2323  O   HOH W 148    13.187  48.467   2.191  1.00 50.09  W O
HET  2324  O   HOH W 149    11.065  34.327   3.436  1.00 50.72  W O
HET  2325  O   HOH W 150    16.314  37.631   3.591  1.00 44.33  W O
HET  2326  O   HOH W 151   -14.021  29.234   2.475  1.00 45.35  W O
HET  2327  O   HOH W 152    -2.913  25.549   3.115  1.00 50.75  W O
HET  2328  O   HOH W 153   -32.162  36.933  -0.013  1.00 49.96  W O
HET  2329  O   HOH W 154   -25.176  57.274  11.637  1.00 35.83  W O
HET  2330  O   HOH W 155    -1.236  62.037   3.918  1.00 52.89  W O
HET  2331  O   HOH W 163   -16.465  38.705  -9.317  1.00 48.95  W O
HET  2332  O   HOH W 164    -9.019  53.609   9.223  1.00 43.37  W O
HET  2333  O   HOH W 165     7.069  43.104   7.087  1.00 35.53  W O
HET  2334  O   HOH W 167    -2.964  56.739 -13.195  1.00 42.67  W O
HET  2335  O   HOH W 168    -0.674  26.977   7.333  1.00 58.51  W O
HET  2336  O   HOH W 169     2.022  62.269 -12.389  1.00 38.09  W O
HET  2337  O   HOH W 160     3.143  33.371  17.461  1.00 35.83  W O
HET  2338  O   HOH W 161    -8.159  47.886 -18.897  1.00 39.24  W O
HET  2362  O   HOH W 162   -25.035  50.827   7.036  1.00 32.68  W O
HET  2363  O   HOH W 163   -24.161  50.362   4.702  1.00 48.13  W O
HET  2364  O   HOH W 164    -0.982  59.064 -13.992  1.00 44.83  W O
HET  2365  O   HOH W 165     8.657  40.987   7.676  1.00 56.40  W O
ATOM    1  C1  LY2 Z   1   -22.659  39.798  -1.719  1.00 32.19  Z C
ATOM    2  C2  LY2 Z   1   -21.941  39.896  -2.932  1.00 31.95  Z C
ATOM    3  C3  LY2 Z   1   -20.613  39.421  -3.017  1.00 31.81  Z C
ATOM    4  C4  LY2 Z   1   -20.004  38.847  -1.880  1.00 31.38  Z C
ATOM    5  C5  LY2 Z   1   -20.712  38.742  -0.656  1.00 31.06  Z C
```

FIGURE 3A-43

```
ATOM      6  C6  LY2 Z   1  -22.045  39.222  -0.584  1.00 31.30  Z C
ATOM      7  C7  LY2 Z   1  -20.042  38.138   0.544  1.00 30.43  Z C
ATOM      8  C8  LY2 Z   1  -19.224  37.014   0.442  1.00 30.47  Z C
ATOM      9  C9  LY2 Z   1  -18.558  36.496   1.562  1.00 30.52  Z C
ATOM     10  C10 LY2 Z   1  -18.711  37.093   2.824  1.00 30.59  Z C
ATOM     11  C11 LY2 Z   1  -19.545  38.214   2.945  1.00 30.25  Z C
ATOM     12  C12 LY2 Z   1  -20.200  38.731   1.814  1.00 29.93  Z C
ATOM     13  O1  LY2 Z   1  -19.087  36.376  -0.778  1.00 30.87  Z O
ATOM     14  C13 LY2 Z   1  -18.362  35.240  -0.950  1.00 30.75  Z C
ATOM     15  C14 LY2 Z   1  -17.643  34.713   0.063  1.00 30.61  Z C
ATOM     16  C15 LY2 Z   1  -17.682  35.335   1.401  1.00 30.77  Z C
ATOM     17  O2  LY2 Z   1  -16.987  34.834   2.277  1.00 31.56  Z O
ATOM     18  N1  LY2 Z   1  -18.471  34.638  -2.293  1.00 30.52  Z N
ATOM     19  C16 LY2 Z   1  -18.695  35.645  -3.345  1.00 30.70  Z C
ATOM     20  C17 LY2 Z   1  -19.209  34.942  -4.608  1.00 31.40  Z C
ATOM     21  O3  LY2 Z   1  -18.262  33.963  -5.029  1.00 31.87  Z O
ATOM     22  C18 LY2 Z   1  -18.027  32.974  -4.029  1.00 31.23  Z C
ATOM     23  C19 LY2 Z   1  -17.486  33.642  -2.755  1.00 30.58  Z C
END
```

Figure 4

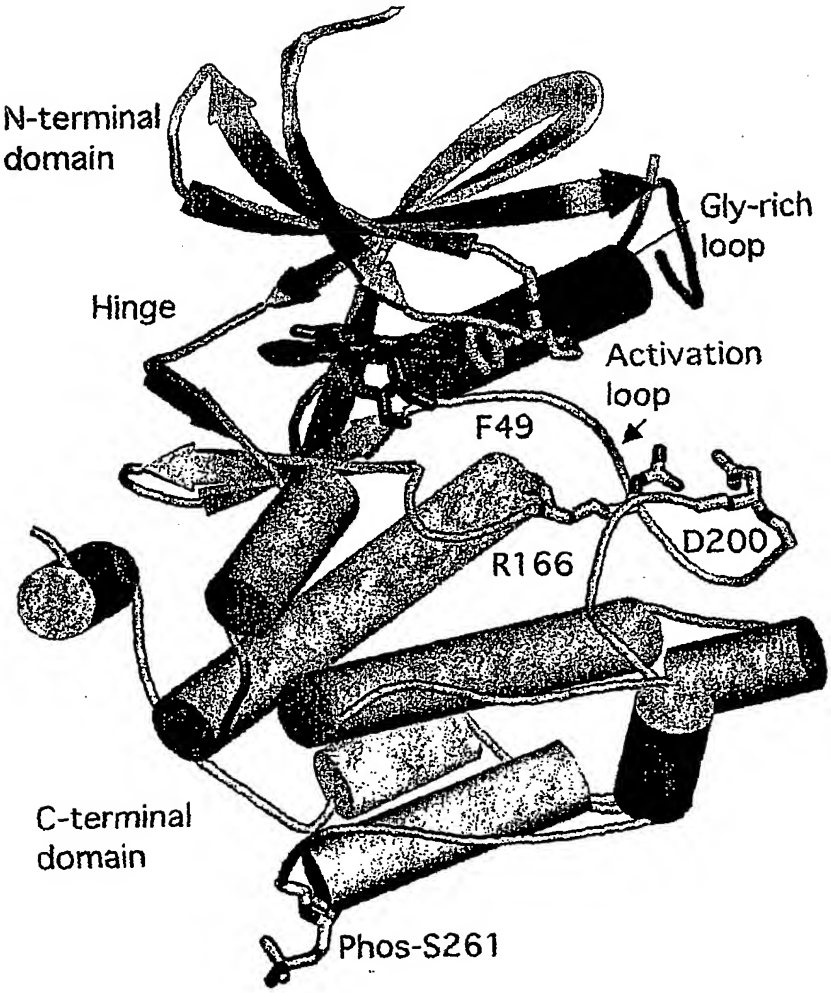
N-terminal domain
Gly-rich loop
Hinge
Activation loop
F49
D200
R166
C-terminal domain
Phos-S261

Figure 5

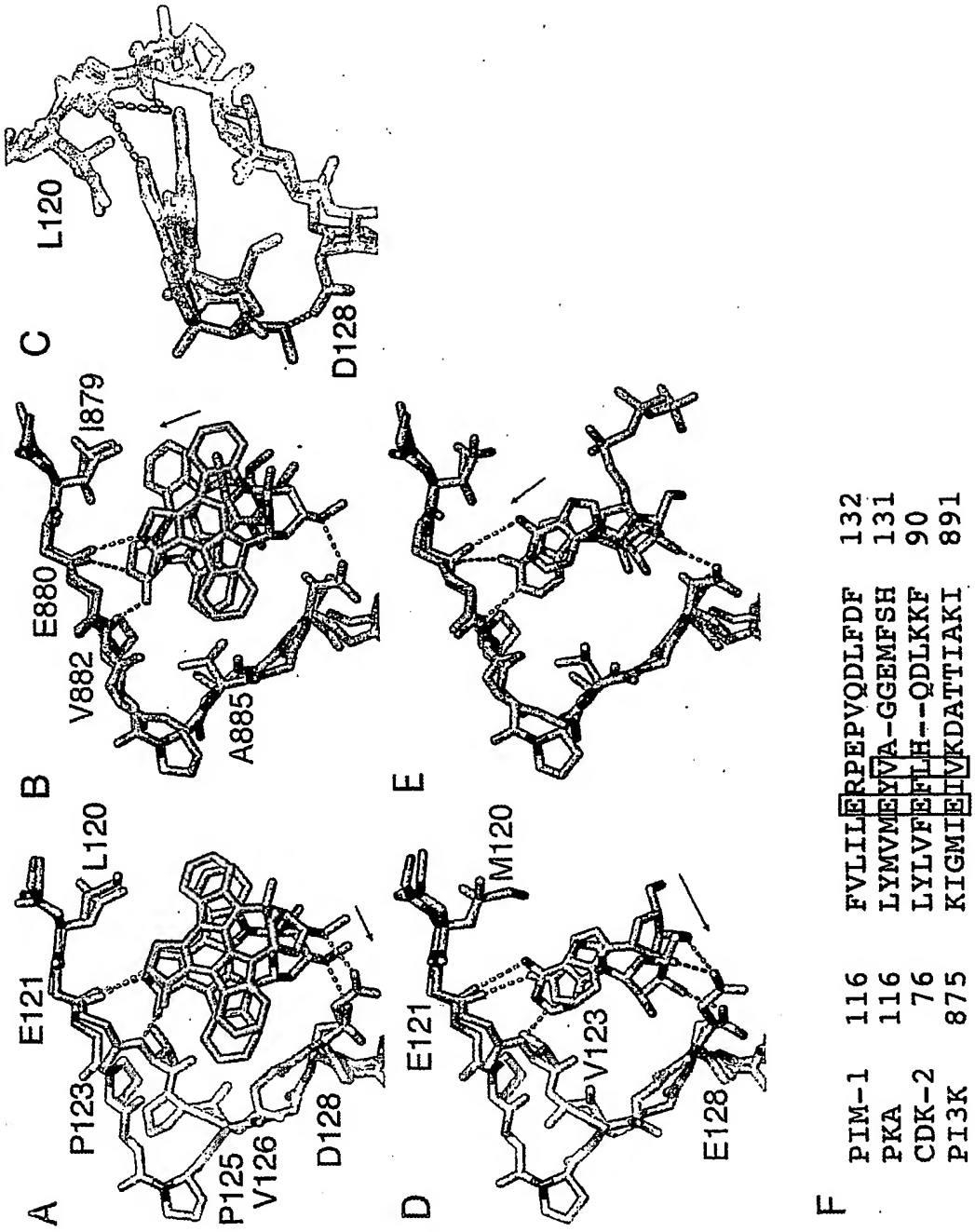
A
E121
L120
P123
P125
V126
D128
B
E880
I879
V882
A885
C
L120
D128
D
E121
M120
V123
E128
E
F
PIM-1 116 FVLILERPEPVQDLFDF 132
PKA 116 LYMVMEYVA-GGEMFSH 131
CDK-2 76 LYLVFEFLH--QDLKKF 90
PI3K 875 KIGMIEIVKDATTIAKI 891

Figure 6

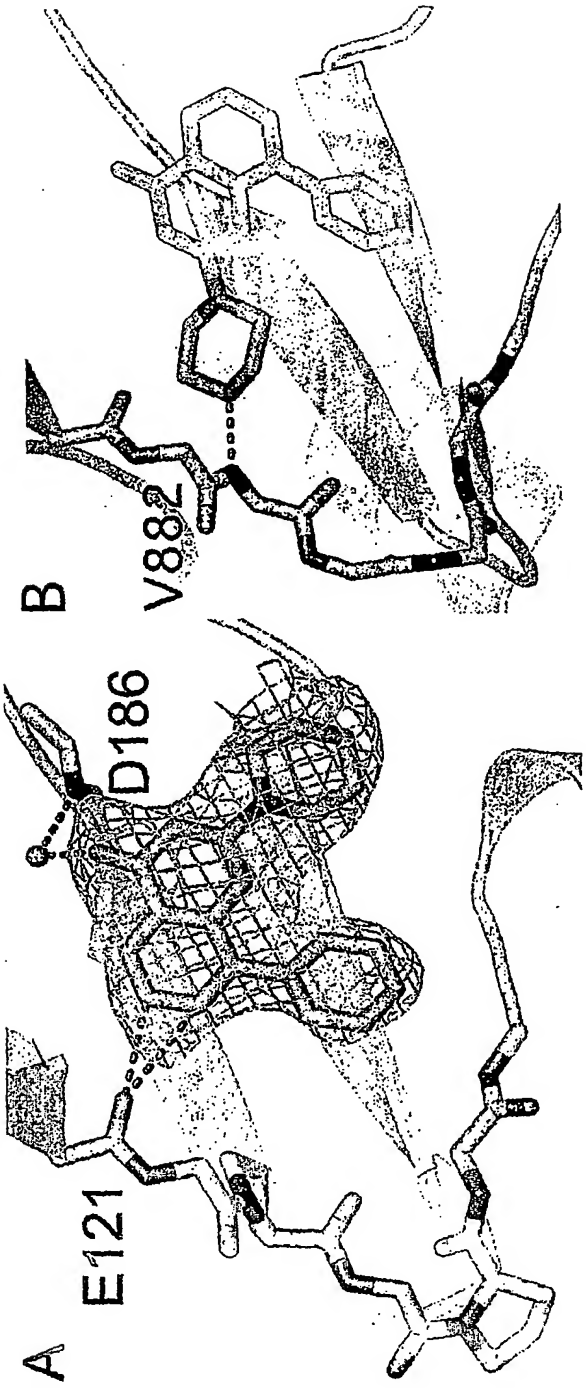

Figure 7

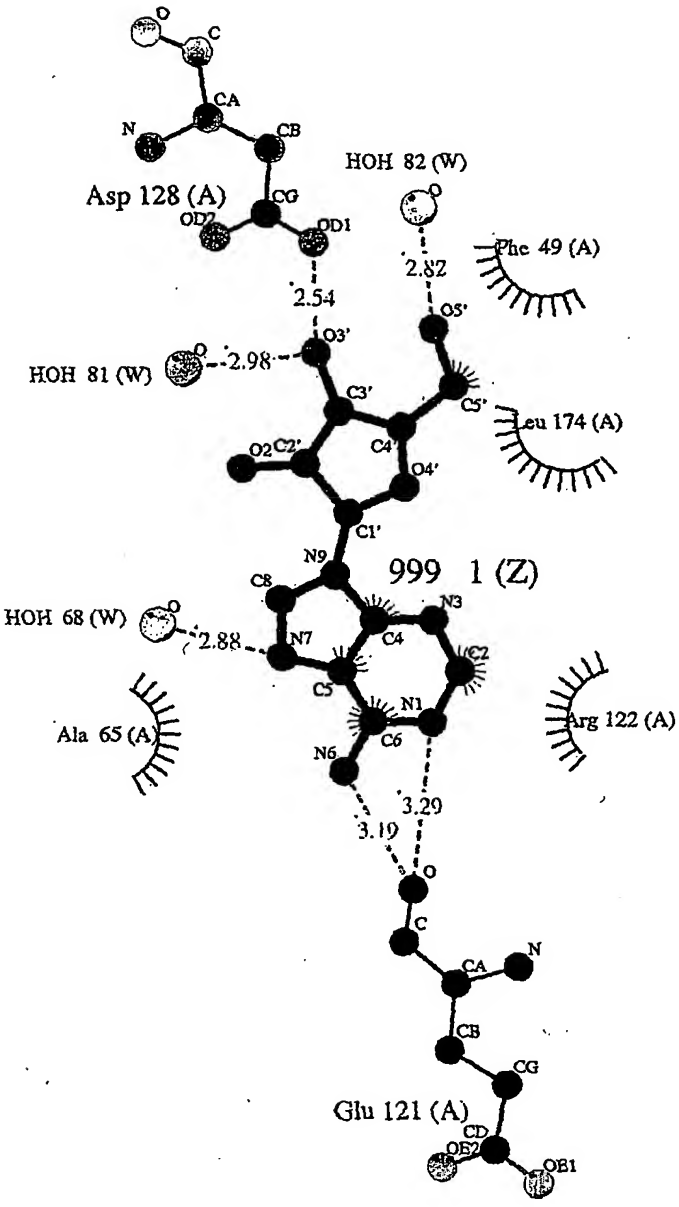
O
C
CA
N
CB
HOH 82 (W)
Asp 128 (A)
CG
OD2
OD1
Phe 49 (A)
2.82
2.54
O5'
O3'
HOH 81 (W)
2.98
C3'
C5'
eu 174 (A)
O2
C2'
C4'
O4'
C1'
N9
999 1 (Z)
C8
N3
HOH 68 (W)
2.88
N7
C4
C2
C5
N1
Ala 65 (A)
Arg 122 (A)
C6
N6
3.29
3.19
O
C
CA
N
CB
CG
Glu 121 (A)
CD
OE2
OE1

Figure 8

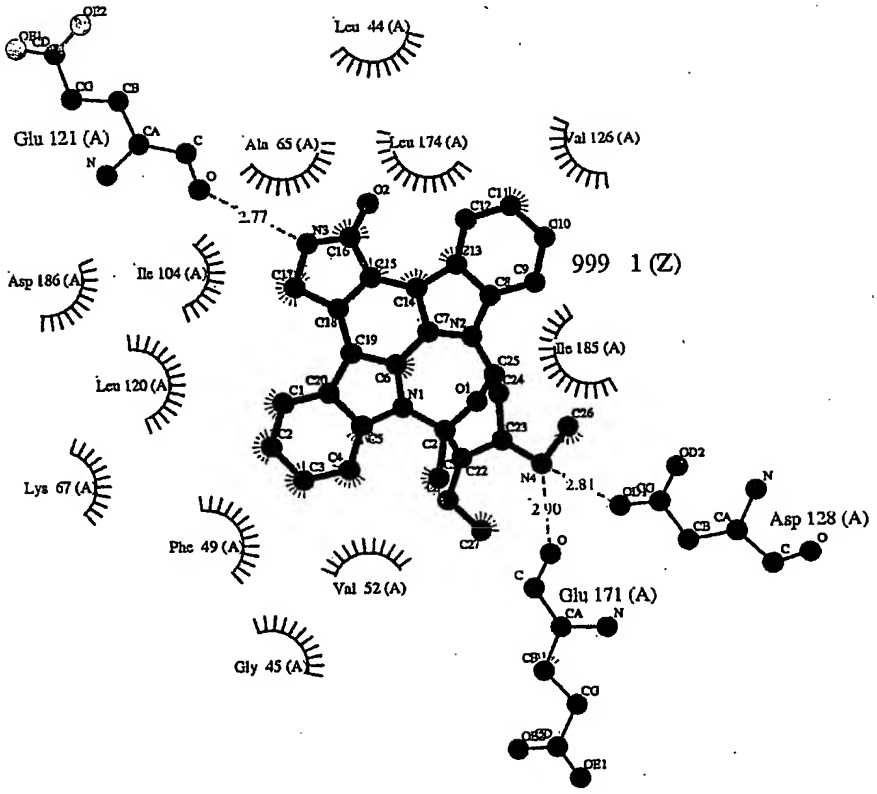
Leu 44 (A)
Glu 121 (A)
Ala 65 (A)
Leu 174 (A)
Val 126 (A)
2.77
999 1 (Z)
Asp 186 (A)
Ile 104 (A)
Ile 185 (A)
Leu 120 (A)
Lys 67 (A)
2.81
2.90
Asp 128 (A)
Phe 49 (A)
Val 52 (A)
Glu 171 (A)
Gly 45 (A)

Figure 9

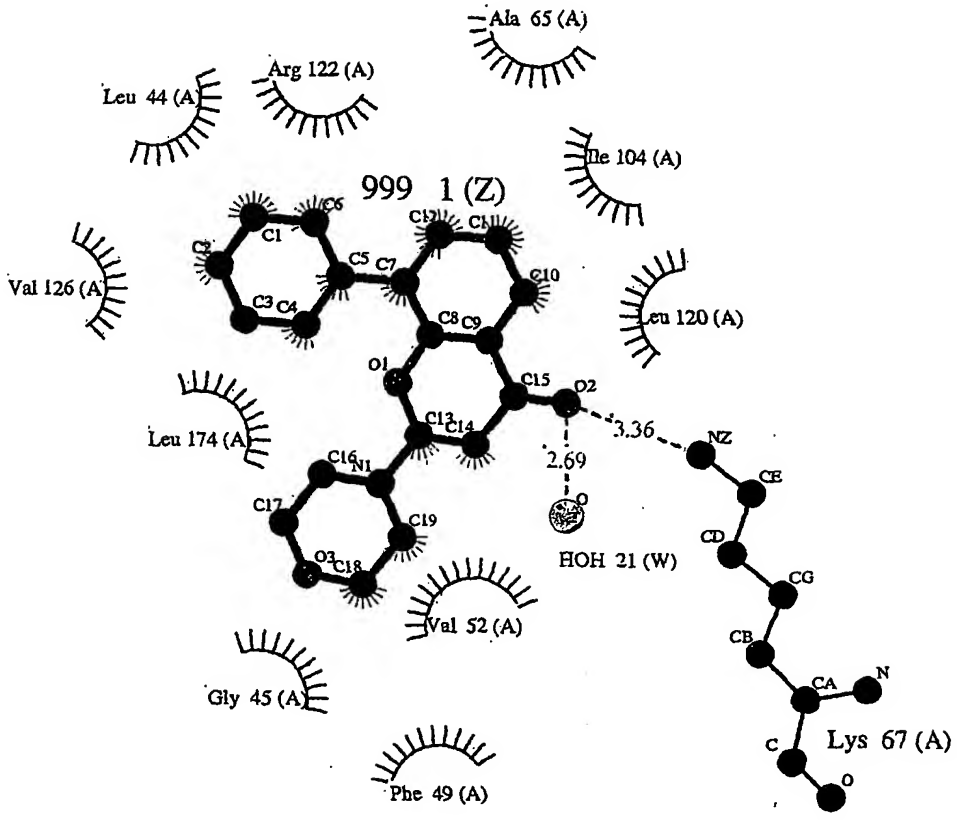
Ala 65 (A)
Arg 122 (A)
Leu 44 (A)
Ile 104 (A)
999 1 (Z)
Val 126 (A)
Leu 120 (A)
Leu 174 (A)
3.36
2.69
HOH 21 (W)
Val 52 (A)
Gly 45 (A)
Phe 49 (A)
Lys 67 (A)

Figure 10

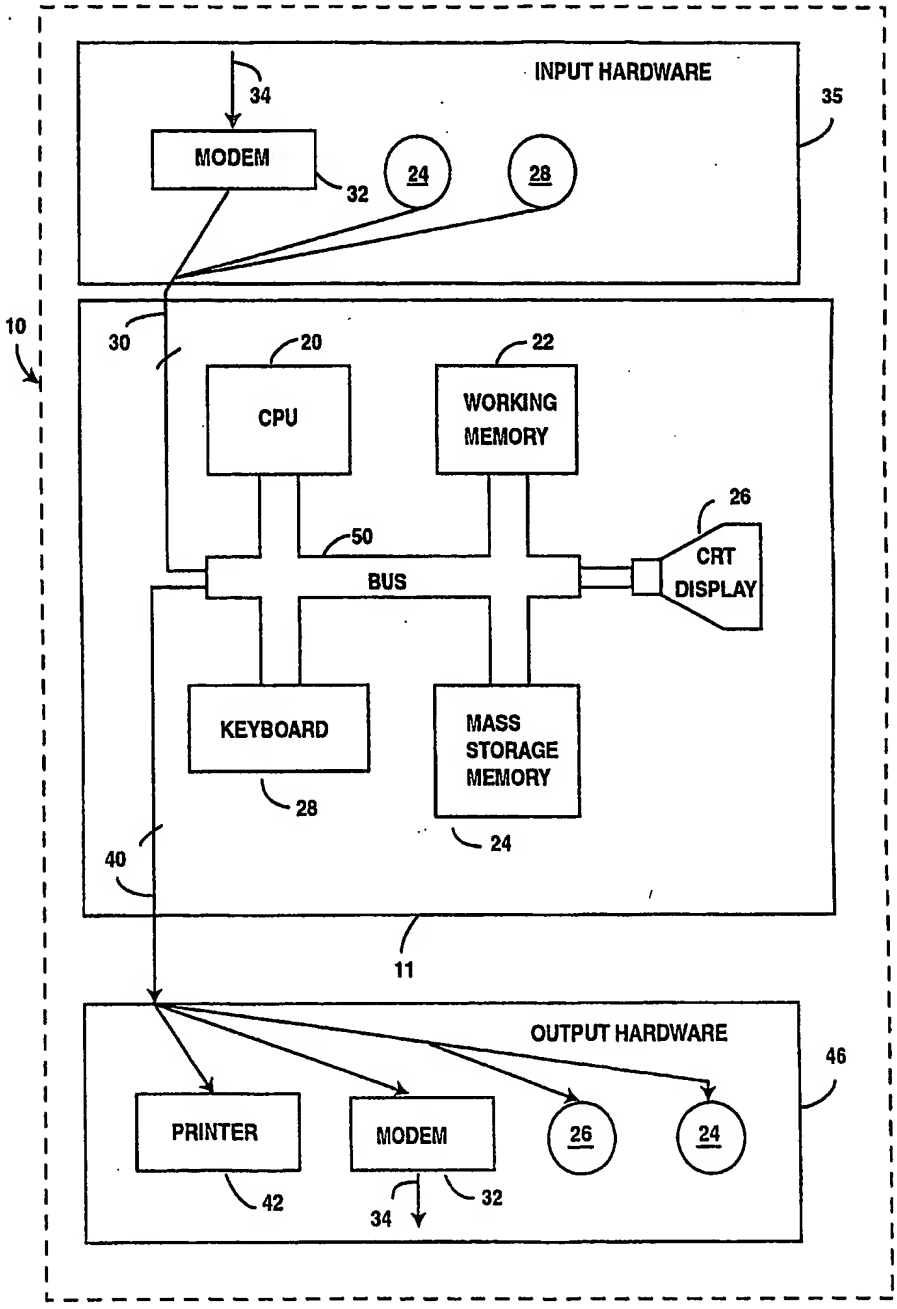
INPUT HARDWARE
35
34
MODEM
32
24
28
10
30
20
22
CPU
WORKING MEMORY
26
50
BUS
CRT DISPLAY
KEYBOARD
28
MASS STORAGE MEMORY
24
40
11
OUTPUT HARDWARE
46
PRINTER
42
MODEM
34
32
26
24

Figure 11

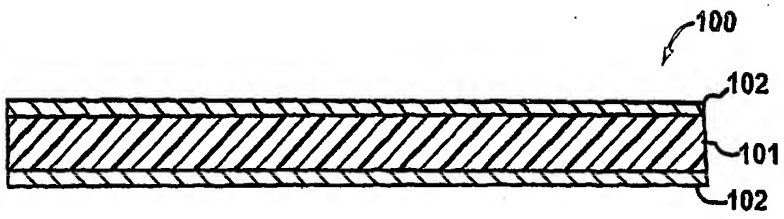

Figure 12